

COM-73-10147

NUMERICAL MODEL FOR THE PREDICTION OF
TRANSIENT WATER QUALITY IN ESTUARY
NETWORKS

James E. Dailey, et al

Massachusetts Institute of Technology

Prepared for:

Office of Sea Grant
Environmental Protection Agency

30 October 1972

DISTRIBUTED BY:

NTIS

National Technical Information Service
U. S. DEPARTMENT OF COMMERCE
5285 Port Royal Road, Springfield Va. 22151

72 12 05 01 COM-73-10147



SEA
GRANT
PROJECT
OFFICE

**NUMERICAL MODEL FOR THE PREDICTION
OF TRANSIENT WATER QUALITY
IN ESTUARY NETWORKS**

by

James E. Dailey

and

Donald R.F. Harleman



Massachusetts Institute of Technology

Cambridge, Massachusetts 02139

**Report No. MITSG 72-15
October 30, 1972**

BIBLIOGRAPHIC DATA SHEET	1. Report No. NOAA-72120501	2.	3. Recipient's Accession No. COM-73-10147
4. Title and Subtitle Numerical Model for the Prediction of Transient Water Quality in Estuary Networks		5. Report Date October 1972	
7. Author(s) James E. Dailey and Donald R.F. Harleman		8. Performing Organization Rept. No. MITSG 72-15	
9. Performing Organization Name and Address Massachusetts Institute of Technology Cambridge, Massachusetts 02139		10. Project/Task/Work Unit No.	
12. Sponsoring Organization Name and Address NOAA, Office of Sea Grant Rockville, Maryland 20852 and Environmental Protection Agency Washington, D. C. 20013		11. Contract/Grant No. S.Gr. GH-88, 2-35150 GFR-800429 (EPA)	
15. Supplementary Notes Massachusetts Institute of Technology Sea Grant Project Office, Report No. MITSG 72-15, 226p., October 1972		13. Type of Report & Period Covered	
16. Abstracts A numerical model is developed for the prediction of transient water quality in an estuary represented as a network of branched and looped, one-dimensional channels. The time scale of the model is of the order of minutes and is called tidal time. Four constituents, salinity, temperature, bio-chemical oxygen demand (BOD), and dissolved oxygen (DO), are included in the mathematical model. In solving the conservation of mass equations for the various water quality constituents, tidal time permits formulation of an ocean boundary condition related to the direction of tidal flow. The numerical solution procedures used in this study are based on the method of weighted residuals, which is an application technique of the finite element method. To demonstrate the predictive capability of the mathematical model, computed results are compared with available data from dye test experiments in the James River Model at the Waterways Experiment Station and with field data obtained from dye tests in Cork Harbour, Ireland. (Author extr.)		14.	
17. Key Words and Document Analysis. Estuaries Water quality Mathematical models Tides Salinity Turbulent diffusion Temperature Dissolved gases Oxygen Numerical analysis		17a. Descriptors Biochemical oxygen demand Mixing Mass transfer Tidal currents Currents Water pollution	
17b. Identifiers/Open-Ended Terms			
17c. COSATI Field/Group 8J; 13B			
18. Availability Statement Released for distribution: <i>Robert R. Freeman</i>		19. Security Class (This Report) UNCLASSIFIED	21. No. of Pages 228
		20. Security Class (This Page) UNCLASSIFIED	22. Price \$ 3.00

**NUMERICAL MODEL FOR THE PREDICTION
OF TRANSIENT WATER QUALITY
IN ESTUARY NETWORKS**

by

James E. Dailey

and

Donald R.F. Harleman

Report No. MITSG 72-15

Index No. 72-315-Ccb

ABSTRACT

A numerical model is developed for the prediction of transient water quality in an estuary represented as a network of branched and looped, one-dimensional channels. A one-dimensional network model is very useful, inasmuch as it can be applied to geometrically complex estuaries which often consist of connected channels and embayments.

The time scale of the model is of the order of minutes and is called tidal time. It is especially important to use tidal time when modeling longitudinal dispersion by numerical techniques. Longitudinal dispersion is a mixing process associated with the tidal motion whereby a constituent is spread out by the interaction of eddy diffusion and the velocity distribution in the channel cross-section. In the non-saline tidal region, the longitudinal dispersion coefficient is a specified function of the instantaneous tidal velocity. Additional dispersion in the salinity intrusion region can be incorporated by using the technique developed by Thatcher and Harleman. Previous one-dimensional network models include empirical parameters which consider the effects of longitudinal dispersion. In general use, however, these parameters must be adjusted in particular applications to match field data.

Four constituents, salinity, temperature, bio-chemical oxygen demand (BOD), and dissolved oxygen (DO), are included in the mathematical model. The concentration distributions of these constituents are obtained by solving sequentially the appropriate conservation of mass equations which include transport, mixing, and reaction processes. Transport processes due to the tidal motion are specified by a combined solution of the continuity and momentum equations including density effects. The reaction processes are characterized by first-order kinetics.

In solving the conservation of mass equations for the various water quality constituents, tidal time permits formulation of an ocean boundary condition related to the direction of tidal flow. On ebb tide, the transport of mass across the ocean boundary is determined by seaward advective flow and the concentration distribution within the estuary. On flood tide, the concentration of a constituent in the inflowing water at the ocean boundary is

prescribed. Previous models require the user to specify the ocean boundary concentration over the entire tidal cycle. Thus, prior knowledge of the boundary concentrations is required in these models in order to achieve the correct seaward movement of the constituent on ebb tide.

The numerical solution procedures used in this study are based on the method of weighted residuals, which is an application technique of the finite element method. Convergence and discretization criteria are developed to aid the user in choosing the mesh spacing and time step.

To demonstrate the predictive capability of the mathematical model, computed results are compared with available data from dye test experiments in the James River Model at the Waterways Experiment Station and with field data obtained from dye tests in Cork Harbour, Ireland. Cork Harbour is used to show the benefits which can be achieved by intermittent rather than continuous injection of wastes near the ocean boundary.

ACKNOWLEDGEMENTS

Primary support for this study came from the Office of Sea Grant, National Oceanic and Atmospheric Administration, U.S. Department of Commerce, Coherent Area Project Grant GH-88 and 2-35150, under the project "Estuary Modeling" (DSR 72602 and 73479) conducted at the Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics of the Department of Civil Engineering.

The final phase of the study was supported by the U.S. Environmental Protection Agency, Grant No. R-800429, under the project "Tidal Variation of Water Quality Parameters in Estuaries" (DSR 73986). This project was administered under the National Coastal Pollution Research Program, National Environmental Research Center, Corvallis, Oregon, by Richard J. Callaway, Project Officer.

Administrative and technical supervision at M.I.T. was provided by Professor Arthur T. Ippen and Professor Donald R. F. Harleman.

Additional support was received for the case study of Cork Harbour, Ireland, from Pfizer International, Incorporated and from Metcalf and Eddy, Incorporated. The authors wish to thank Mr. John Podger, Mr. Jekabs Vittands, and Mr. Richard Sherman of Metcalf & Eddy, Incorporated, for their helpful assistance. The dye test results were made available by Mr. Ferdinand Veith of Pfizer International, Incorporated, and Dr. David Cook of Raytheon, Incorporated, helped resolve questions about them. Data for the James River Model Study was assembled with the assistance of Mr. Robert A. Boland of the U. S. Army Corps of Engineers, Waterways Experiment Station.

The major part of the computer work was done at the M.I.T. Information Processing Service Center. Special appreciation is extended to Mr. Eric Wood, Research Assistant, for his assistance in the development of the computer programs for the hydraulic computations and for the time spent in grappling with computational problems which arose. Schematization and drafting work was performed by Mr. John Whelan, Mr. Stephen Doret, Mr. Gerard Lum, and Mr. Michael Ryan. Mrs. Stephanie M. Demeris did an exceptionally conscientious job in typing the text.

TABLE OF CONTENTS

	Page
ABSTRACT	2
ACKNOWLEDGEMENTS	4
TABLE OF CONTENTS	5
LIST OF FIGURES	8
LIST OF TABLES	11
LIST OF SYMBOLS	12
I. INTRODUCTION	19
1.1 Mathematical Models and the Estuarine Environment	19
1.2 Summary of the Present Study	23
II. THEORETICAL CONSIDERATIONS	27
2.1 Governing Equations and Assumptions	27
2.1.1 One-Dimensional Conservation of Mass Equation	27
2.1.2 Continuity Equation for Water	30
2.1.3 Longitudinal Momentum Equation Including Density Effects	33
2.2 Review of Existing Water Quality Models	36
2.2.1 Non-Tidal Advective Models	37
2.2.2 FWQA Dynamic Estuary Model	40
2.2.3 Lagrangian Method of H.B. Fischer	46
2.2.4 Tidal Time Models of Lee and Harleman and of Thatcher and Harleman	49
2.2.5 Finite Element Approaches	53
2.2.5a The Method of Weighted Residuals	56
2.2.5b Variational Techniques	57
2.3 Formulation of a New Approach to the Network Problem	59
2.3.1 Areas of Application	59
2.3.2 Evaluation of Existing Techniques	63
2.3.3 The Ocean Boundary Condition	67
2.3.4 Solution Technique for Multiple Constituents	72

	Page
III. DEVELOPMENT OF THE NUMERICAL SOLUTION TECHNIQUE	81
3.1 Conservation of Mass Equation	81
3.1.1 Application of the Method of Weighted Residuals	81
3.1.2 Initial Conditions and Boundary Conditions	92
3.1.3 Mass Conservation Properties	96
3.1.4 Convergence Criteria	101
3.1.5 Discretization Criteria	108
3.1.6 Tests of the Discretization Criteria	113
3.2 Continuity and Momentum Equations	127
3.2.1 Finite Element, Implicit Scheme of Gunaratnum and Perkins	127
3.2.2 Initial Condition and Boundary Conditions	136
3.2.3 Discretization Criteria	137
IV. PROGRAMMING CONSIDERATIONS	139
4.1 Network Formulation	139
4.2 Method of Superposition	140
4.3 Solution Procedure for Water Surface Elevations and Discharges	141
4.3.1 Interior Mesh points	142
4.3.2 Boundary Mesh Points	144
4.4 Solution Procedure for Concentrations	148
4.4.1 Interior Mesh Points	149
4.4.2 Boundary Mesh Points	151
V. CASE STUDIES	155
5.1 Hydraulic Model of the James River at the U.S. Army Corps of Engineers Waterways Experiment Station	155
5.1.1 Geometry and Schematizations	158
5.1.2 Verification of the Tidal Hydraulics	161
5.1.3 Dye Test Simulations	169

	Page
5.2 Cork Harbour, Ireland	185
5.2.1 Geometry and Schematizations	186
5.2.2 Verification of the Tidal Hydraulics	187
5.2.3 Dye Test Simulation	191
5.2.4 Simulation of Alternative Waste Disposal Schemes	198
VI. SUMMARY AND CONCLUSIONS	210
REFERENCES	214
APPENDICES	218
A. SUMMARY OF INTEGRAL VALUES IN THE WEIGHTED RESIDUAL EQUATIONS	218
B. SPECTRAL DENSITY OF THE CONCENTRATION RESPONSE TO AN INSTANTANEOUS INJECTION OF MASS	220

LIST OF FIGURES

Figure		Page
1.1	Schematic Diagram of a Typical Estuary with Multiple Waste Inputs	25
2.1	Computational Molecule for the Stone and Brian Scheme	49
2.2	Computational Grid in Space and Time for the Tidal Hydraulics and Water Quality Models of Lee and Harleman	50
2.3	Definition Sketch for Finite Difference Method	54
2.4	Definition Sketch for Finite Element Method	55
2.5	Interpolating Function $\Phi_j(x)$ for a Piecewise Linear Approximation	55
2.6	Schematic Map of Cork Harbour, Ireland	61
2.7	Time Variation of Boundary Discharge and Concentration	70
2.8	Major Features of the Nitrogen Cycle	73
3.1	Linear Variation of the Equation Terms over the Elements	81
3.2	Simply Supported Beam Analogy	84
3.3	Velocity Factor ϕ for $\alpha = 0$ and $\gamma = 0$	106
3.4	Velocity Factor ϕ for $\beta = 1$ and $\gamma = 0$	107
3.5	Normalized Spectral Density $^0S(\omega, x)$	110
3.6	5% Cutoff $\frac{4\omega E}{U}$ with Zero Decay	112
3.7	Propagation of a Steep Front	118
3.8	Comparison of Analytical Solution and Numerical Solution with $\Delta x = 1000$ ft. and Greater, and $\Delta t = 465.75$ sec.	123
3.9	Effect of Increasing Δx to 2000 ft. and Greater	124

Figure		Page
3.10	Effect of Increasing Δt to 1863 sec.	125
3.11	Effect of Increasing Δt to 1863 sec. and Δx to 2000 ft. and Greater	126
4.1	Example Network	139
5.1	Location Map of the James River	156
5.2	Loop Section of the James River between Richmond and Hopewell	157
5.3	Reach-Node Representation of the James River	159
5.4a	Tidal Stage at Hampton Roads Gage, 11,5000 cfs Test	164
5.4b	Tidal Stage at Hampton Roads Gage, 1000 cfs Test	164
5.5a	Tidal Stage at Scotland Gage, 11,500 cfs Test	165
5.5b	Tidal Stage at Scotland Gage, 1000 cfs Test	165
5.6a	Tidal Stage at Weyanoke Gage, 11,500 cfs Test	166
5.6b	Tidal Stage at Weyanoke Gage, 1000 cfs Test	166
5.7a	Tidal Stage at VEPCO Gage, 11,500 cfs Test	167
5.7b	Tidal Stage at VEPCO Gage, 1000 cfs Test	167
5.8	Concentration Increase near VEPCO, 1000 cfs Test	172
5.9	Concentration Increase in Curles Neck Loop, 1000 cfs Test	173
5.10	Concentration Increase in Turkey Island Loop, 1000 cfs Test	174
5.11	Concentration Increase near Hopewell, 1000 cfs Test	175
5.12	Concentration Increase near VEPCO, 11,500 cfs Test	178
5.13	Concentration Increase in Curles Neck Loop, 11,500 cfs Test	179

Figure		Page
5.14	Concentration Increase in Turkey Island Loop, 11,500 cfs Test	180
5.15	Concentration Increase near Hopewell, 11,500 cfs Test	181
5.16	Concentration Increase in the Appomattox River at Hopewell, 11,500 cfs Test	182
5.17	Concentration Increase near Weyanoke Point, 11,500 cfs Test	183
5.18	Concentration Increase in the Chickahominy River, 11,500 cfs Test	184
5.19	Computed Water Surface Elevations in Cork Harbour	189
5.20	Computed Discharges in Cork Harbour	190
5.21	Vertical Profile Stations for Ballybricken Dye Injection	192
5.22	Dye Concentration versus Time at Stations B and D, Cork Harbour	197
5.23	Concentration Profiles in Reach 1, Tidal Cycle 14	201
5.24	Concentration Profiles in Reach 2, Tidal Cycle 14	202
5.25	Concentration Profiles in Reach 3, Tidal Cycle 14	203
5.26	Concentration Profiles in Reach 4, Tidal Cycle 14	204
5.27	Concentration Profiles in Reach 5, Tidal Cycle 14	205
5.28	Concentration Profiles in Reach 6, Tidal Cycle 14	206
5.29	Concentration Profiles in Reach 7, Tidal Cycle 14	207
5.30	Concentration Profiles in Reach 8, Tidal Cycle 14	208
B.1	Evaluation of $\text{rcos}\theta$ as a Function of $\frac{4\sigma E}{U^2}$ and $\frac{4KE}{U^2}$	223

LIST OF TABLES

Table		Page
3.1	Discretization Parameters for Propagation of a Steep Front	116
3.2	Computational Mesh for Propagation of a Steep Front	117
4.1	Connectivity of Example Network	140
5.1	Constant Fresh Water Inflows for the James River Model in Prototype Units	161
5.2	James River Model Schematization Parameters in Model Units	163
5.3	Cork Harbour Schematization Parameters	188
5.4	Predicted Tidal Stages for the Period of the Ballybricken Dye Test	194
5.5	Base Flows in the River Lee	195

LIST OF SYMBOLS

An attempt to draw together the literature from different areas inevitably produces conflicts in notation. The same symbol is often used to describe many different quantities. Where such a symbol is widely accepted as denoting a well-known quantity, no attempt is made to change it simply to achieve a conflict-free notation. The definition which applies at any given point in the text should be clear from the context in which the symbol is used.

A	cross-sectional area of a channel
$\bar{A}$	time averaged A over a period (Eqn. 2.23)
A_i	cross-sectional area of channel i (Eqn. 2.24)
A_j^*	surface area of a junction (Eqn. 2.27)
A_j^n	discrete area at mesh point j and time step n
A_s	slack tide channel area (Eqn. 2.24)
A_ω	Fourier series coefficient (Eqn. 3.37)
$\underline{A}$	coefficient matrix for a set of simultaneous equations
$\underline{A}'$	coefficient matrix for interior mesh points of hydraulic and water quality solution procedures
B	topwidth of a channel
B_o	linearized topwidth (Eqn. 3.65)
B_{core}	width of channel core area (Eqn. 2.19)
B_i	right-hand side element for water quality mesh point equations (Eqn. 4.7)
B_i^n	discrete topwidth at mesh point i at time step n

B_{core}	width of channel core area (Eqn. 2.19)
B_{storage}	width of channel storage area (Eqn. 2.19)
C	dissolved oxygen (DO) concentration
C_s	saturation concentration of dissolved oxygen
C_z	Chezy coefficient
D	dissolved oxygen deficit $C_s - C$
D_1^N, D_2^1	right-hand sides for boundary equations in network solution procedure
$\underline{D}$	tridiagonal coefficient matrix (Eqn. 3.17)
E	longitudinal dispersion coefficient $E(x,t)$
E_j^n	discrete longitudinal dispersion coefficient at mesh point j and time step n
$\bar{E}$	time averaged E over a period (Eqn. 2.23)
E_s	slack tide dispersion coefficient (Eqn. 2.24)
E_T	Taylor dispersion coefficient, $77n U R_h^{5/6}$
F	Froude number, $\frac{U}{\sqrt{\frac{A}{g_B}}}$
$H(\omega, x)$	complex frequency response for convective diffusion equation with decay
I	mass injection rate (Eqn. 3.56)
K	decay coefficient in conservation of mass equation, dispersion parameters (Eqn. 2.33)
K_d	eddy diffusion coefficient (Eqn. 2.30)
K_T	heat loss coefficient (Eqn. 2.3)
K_{ij}	decay of constituent i due to unit concentration of constituent j (Eqn. 2.46)
K_o	exponential rate constant for decrease of ocean boundary concentration

K_1	BOD decay rate (Eqn. 2.4)
K_2	reaeration coefficient (Eqn. 2.5)
L	biochemical oxygen demand (BOD) concentration (Eqn. 2.4), harmonic wave length in a Fourier series (Eqn. 3.37), length of an estuary (Eqn. 2.33)
L_L	BOD concentration of a lateral inflow
$L(\zeta)$	differential operator (section 2.2.5a)
M	number of water quality mesh points in a channel
ΔM_a	parcel of mass transferred by advection (Eqn. 2.29)
ΔM_d	parcel of mass transferred by diffusion or dispersion (Eqns. 2.30 and 2.32)
N	number of hydraulic mesh points in a channel
P_L, P_R	reactions for a simply supported beam (Fig. 3.2)
Q	discharge $Q(x,t)$
Q_b	discharge at the ocean boundary (Eqn. 2.39)
Q_f	fresh water throughflow
Q_j	flow into junction j (Eqn. 2.27)
Q_j^n	discrete discharge at mesh point j and time step n
$Q^0(j)$	null solution for Q at mesh point j (Eqn. 4.1)
Q_L	point lateral inflow
R	residual difference between partial differential equation and piecewise continuous approximation (Eqn. 2.36)
R_1	damping ratio (Eqn. 3.41)
R_2	wave celerity ratio (Eqn. 3.42)
S	lumped source term for conservation of mass equations
$S(\omega, x)$	spectral density for convective diffusion equation with decay
$^0S(\omega, x)$	normalized spectral density
S_f	friction slope, $\frac{Q Q }{A^2 C_z^2 R_h}$

T	tidal period, period of a Fourier harmonic, temperature (Eqn. 2.3), distance travelled by a volume element (Eqn. 2.32)
T^e	temperature excess $T - T_e$
T_e	equilibrium temperature (Eqn. 2.3)
U	mean discharge velocity, $\frac{Q}{A}$
U_o	linearized velocity (Eqn. 3.72b)
U_f	net advective flow velocity (Eqn. 3.55)
U_T	amplitude of tidal velocity (Eqn. 3.55)
$a(x)$	local tide range (Eqn. 2.12)
a^i	coefficient matrix main diagonal element (Eqn. 3.17)
$a_1^i, a_2^i, a_3^i, a_4^i$	coefficient matrix lower diagonal submatrix element (Eqn. 3.70)
b^i	coefficient matrix lower diagonal element (Eqn. 3.17)
$b_1^i, b_2^i, b_3^i, b_4^i$	coefficient matrix main diagonal submatrix elements (Eqn. 3.70)
c	concentration of water quality constituent, small amplitude wave celerity
$\bar{c}$	concentration averaged over a tidal period (Eqn. 2.23)
c^*	representative concentration in the FWOA Model (Eqn. 2.29)
c_o	mixed concentration of injection and fresh water flow (Eqn. 3.56), linearized wave celerity (Eqn. 3.72b)
c_b	concentration at the ocean boundary (Eqn. 2.39)
c_j	concentration at junction j (Eqn. 2.31)
$\bar{c}_j^n$	discrete concentration at mesh point j at time step n
$\bar{\underline{c}}$	vector of discrete mesh point concentrations
c_ℓ	concentration of the longer volume element (Eqn. 2.32)
c_s	slack tide concentration (Eqn. 2.24), concentration of the shorter volume element (Eqn. 2.32)
c^i	coefficient matrix upper diagonal element (Eqn. 3.17)

$c_1^i, c_2^i, c_3^i, c_4^i$	coefficient matrix upper diagonal submatrix elements (Eqn. 3.70)
$\bar{c}_i$	concentration at node i in water quality network solution procedure (Eqn. 4.11)
d_c	depth to the centroid of a channel cross-section
$\underline{d}$	right-hand side vector (Eqn. 3.71)
d_a^i, d_b^i, d_c^i	right-hand side coefficient matrix elements (Eqn. 3.17)
d_1^i, d_2^i	right-hand side vector elements (Eqn. 3.70)
$dx_1(j), dx_2(j), dx_3(j), dx_4(j), dx_M(j),$ $dx_{11}(j), dx_{22}(j), dx_{33}(j), dx_{44}(j)$	influence coefficients at mesh point j for hydraulic and water quality network solution procedures
$\underline{e}$	right-hand side vector (Eqn. 3.17)
$f_1^{i,n}, f_2^{i,n}, f_3^{i,n}, f_4^{i,n}$	equation factors (Eqn. 3.17)
g	acceleration of gravity
i	$\sqrt{-1}$, mesh point index
j	mesh point index
k	frictional resistance coefficient (Eqns. 2.26 & 3.69), element of complex constant ξ (Eqn. 3.38)
l_i	length of channel i (Eqn. 2.28)
l_s	length of the shorter volume element (Eqn. 2.32)
n	Manning resistance coefficient, time step index
$p(x)$	distributed load (Fig. 3.2)
q	element of complex constant ξ (Eqn. 3.38)
q_L	lateral inflow per unit length of a channel
r	per cent return at the ocean boundary (Eqn. 2.40), element of complex constant ξ (Eqn. 3.38), spectral density parameter (Eqn. 3.49)
r_e	time rate of external addition of mass per unit volume (Eqn. 2.1)

r_i	time rate of internal addition of mass per unit volume (Eqn. 2.1)
r_o	spectral density parameter (Eqn. 3.49)
s	salinity concentration, element of complex constant ξ (Eqn. 3.38)
s_o	ocean salinity concentration (Eqn. 2.33)
$\frac{s}{s_o}$	dimensionless salinity concentration $\frac{r}{r_o}$ (Eqn. 2.33)
t	time variable
t_{HWS}	time of high water slack tide
t_{LWS}	time of low water slack tide
w_i	weighting functions for the method of weighted residuals (Eqn. 2.37)
x	longitudinal distance variable
$\frac{x}{L}$	dimensionless distance $\frac{x}{L}$ (Eqn. 2.33)
z	water surface elevation $z(x,t)$
z_j^n	discrete water surface elevation at mesh point j and time step n
$z^0(j)$	null solution for z at mesh point j
$z_o(x)$	local mean water surface elevation (Eqn. 2.12)
Γ^i	coefficient matrix upper diagonal submatrix (Eqn. 2.47)
$\Delta_{j,j+1}$	length of an element between mesh points j and $j+1$
Λ^i	coefficient matrix main diagonal submatrix (Eqn. 2.47)
T^i	coefficient matrix lower diagonal submatrix (Eqn. 2.47)
$\Phi_j(x)$	interpolating functions involving mesh point j (Eqn. 2.35)
α	$\frac{E\Delta T}{\Delta x^2}$ (Eqn. 3.43)
$\alpha_1, \alpha_2, \alpha_3, \alpha_4$	equation coefficients for hydraulic network solution procedure (Eqn. 4.3a)

$\alpha_{11}, \alpha_{1M}, \alpha_{M1}, \alpha_{MM}$	equation coefficients for water quality network solution procedure (Eqn. 4.10)
$\beta \quad \frac{U\Delta t}{\Delta x}$	(Eqn. 3.43)
$\beta_1, \beta_2, \beta_3, \beta_4$	equation coefficients for hydraulic network solution procedure (Eqn. 4.3b)
β_1, β_M	right-hand side entries for water quality network solution procedure (Eqns. 4.10)
γ	$K\Delta t$ (Eqn. 3.43)
$\delta(x)$	Dirac delta function
δ_{ij}	Kronecker delta
ζ	arbitrary dependent variable (Fig. 2.3)
$\zeta_j(t)$	discrete value of ζ at mesh point j as a function of time (Eqn. 2.35)
η_1	dispersive flux into upstream boundary (Eqn. 3.15a)
η_M	dispersive flux into downstream boundary (Eqn. 3.15b)
θ	spectral density parameter (Eqn. 3.4a)
θ_s	time shift (Eqn. 3.55)
λ	$U \pm c$
$\bar{\lambda}$	$U \mp c$
$\lambda_1^{i,n}$	$(U + c)_i^n$
$\lambda_2^{i,n}$	$(U - c)_i^n$
ξ	complex constant in the series approximation of difference equation
ρ	density of water
σ	angular frequency $\frac{2\pi}{T}$
$\tau(x)$	phase lag (Eqn. 2.12)
ϕ	velocity factor in series approximation of difference equations
ψ	right-hand side for the hydraulics weighted residuals equations

CHAPTER I

INTRODUCTION

1.1 Mathematical Models and the Estuarine Environment

Water quality degradation has become a matter of concern as estuaries receive growing amounts of waste from industries and municipalities located on their shores. In predicting the effectiveness of various water quality control measures, planners have made increasing use of mathematical models which are usually executed in the form of computer programs. Physical models are of limited use for estuarine water quality studies because of the difficulty of simulating reaction processes at reduced scale. In addition, their high distortion ratios (usually a factor of 10 to 1) prevent them from achieving mass transfer similitude. Field data is expensive to collect, and usually it cannot be used in a predictive role if the regime of the estuary will be changed by the planned control measures.

To be used in a predictive role, a mathematical model must reproduce the natural processes which occur in the prototype estuary. Transport processes which include the advection and dispersion of a substance are governed by the tidal motion of the estuary. The tidal motion may be characterized as unsteady, non-uniform, free surface flow, which results from the interaction of tidal excitation by the ocean and fresh water flow from upland rivers. Near the ocean entrance of an estuary, the cross-sectional velocity distribution of the tidal flow is modified by the intrusion of denser saline water from the ocean. This intrusion of salinity creates internal density currents which have a significant

effect on the mixing behavior of the estuary. In estuaries where turbulent energy for mixing comes primarily from velocities generated by the tidal motion, the water mass becomes mixed, and salinity gradients exist in both the longitudinal and vertical directions. Such estuaries are found typically on the east and west coasts of the United States. In the lower Mississippi River where tidal currents are weak, the flow is highly stratified and the saline water intrudes along the bottom as a wedge.

Less well-established in mathematical modeling than the transport processes are the reaction processes. These deal with the addition and removal of a constituent, either within the water mass or across its boundaries. If the constituent is dissolved oxygen (DO), it may be consumed within the water mass by bio-chemical oxygen demand (BOD) and be replenished by transfer across the water surface from the atmosphere. BOD and DO are the classical water quality parameters used in the field of sanitary engineering. In the past, it was assumed on experimental evidence that constituents such as BOD undergo a so-called first order reaction where the rate of removal of constituent is proportional to the amount present. This assumption, when applied to steady state conditions in river-like flow, permitted a straightforward solution of the water quality problem in the form of the Streeter-Phelps equations. With the advent of the digital computer, it is possible now to consider several constituents simultaneously and complex reaction processes which may be highly non-linear. Research is progressing to find more descriptive sets of water quality parameters and to define the reactions and interactions between them.

To be most exact, a mathematical model of a given estuary should consider all three space dimensions and time. Pritchard has derived the set of governing equations in Chapter II of TRACOR (1971), but several of the solution parameters have not been evaluated by research. Therefore, some simplifying assumptions are required. If a three-dimensional model were available, it would require lengthy computational time on a very large computer. Faced with the task of solving real-world water quality problems, analysts have made appropriate assumptions for particular classes of estuaries. The usual approach has been to average over one or two of the space dimensions. For shallow bays, Leendertse (1971) and Shankar and Masch (1970) have developed models which are vertically averaged and thus consider the two horizontal space dimensions and time. Several analysts have approached the problem of salinity intrusion in the vertical and longitudinal dimensions, assuming that the estuary is laterally homogeneous.

One-dimensional, water quality models have been developed for single-channel estuaries. The state-of-the-art of these models has been reviewed by Harleman in Chapter II of TRACOR (1971). The basic assumption of these one-dimensional models that quantities such as velocity and concentration are uniform across the estuary cross-section is seldom met; however, such models have been applied with good results. Their particular advantage is that their data requirements are concise and closely related to information available in the field.

One-dimensional network models are more useful than single channel models and two-dimensional, vertically mixed models. They can be applied

to geometrically complex estuaries, which often consist of channels and embayments connected in some arbitrary manner. For channelized estuaries, such as the Sacramento-San Joaquin Delta, Feigner and Harris (1970), and Fischer (1970) describe mathematical models which can handle a network of one-dimensional channels.

A one-dimensional model must account for both the advection of constituents by the mean discharge velocity and the spreading of the concentration profile by longitudinal dispersion. Longitudinal dispersion results from the interaction of eddy-diffusion and the shear-induced velocity distribution across the channel cross-section. This process is especially important in the region of salinity intrusion where the mixing process is heightened by density currents and in areas where steep concentration fronts may exist due to intermittent injection schedules. Existing one-dimensional network models include empirical parameters which consider the effects of longitudinal dispersion. In general, these parameters must be adjusted in particular applications to match field data.

In formulating a mathematical model for estuarine water quality it is necessary to specify conditions at the boundaries. This is straightforward at upstream boundaries, where either known concentration or mass flux can be prescribed. At the ocean boundary, however, the problem is more difficult, especially on ebb tide when there is no physical constraint on the movement of a constituent out of the estuary. Many existing models require the user to specify the ocean boundary concentration over the entire tidal cycle. This has the effect of specifying the amount of mass leaving the estuary, which may or may not match the amount

of mass being advected toward the ocean boundary. In applications where the ocean boundary concentration is important the user must have an accurate estimate of the results before the modeling procedure begins.

1.2 Summary of the Present Study

The mathematical model developed in this study is applicable to unsteady flow in branched and looped networks of one-dimensional channels. The time scale considered is of the order of minutes so that instantaneous turbulent fluctuations of velocity and concentration are averaged out. However, the remaining variation over a tidal cycle of about 12 hours is reasonably continuous. This time scale has been called "tidal time" by Thatcher and Harleman (1972). It is especially important to use tidal time when modeling the longitudinal dispersion process. Turbulent energy for mixing is supplied by the time-varying tidal flows, and this mixing combined with advection on flood tide results in net movement of a constituent about one tidal excursion upstream of the injection point. Non-tidal advective models can achieve such upstream movement only by artificially increasing longitudinal dispersion. Tidal time also permits the specification of boundary conditions at the ocean entrance which are related to the direction of the tidal flow. On ebb tide, advection of a constituent out of the estuary is relatively unrestricted; however, inward advection on flood tide is prescribed. In this way, the effects of tidal flushing are reproduced. With the use of tidal time it is also possible to consider intermittent injection schemes which use the benefits of tidal flushing by placing the bulk of a waste in the water mass which leaves the estuary on ebb tide.

Four constituents, salinity, temperature, BOD, and DO are included in the model as shown in Figure 1.1. These are the constituents which are commonly considered in current engineering practice. The distribution of each constituent in tidal time is obtained by solving sequentially the appropriate conservation of mass equations which include the transport, mixing and reaction processes. To specify the transport process, the tidal hydraulics are established first by a combined solution of the continuity and momentum equations. Included are the effects of density gradients on momentum transport which are associated with the salinity distribution. The reaction processes are assumed to be first order, with the amount of constituent added or removed proportional to the amount present. The mathematical formulation of the model does not depend on this assumption. More complex interactions of constituents may be specified when the reaction processes are better defined.

Inasmuch as the mathematical model is a numerical solution of a set of partial differential equations, the accuracy of its results depends upon correct treatment of the boundary conditions and how well it converges to the exact concentration distribution. Convergence of the numerical solution is a function of the computational mesh spacing Δx and the time step Δt of the calculations. Discretization criteria are developed to serve as a guide in choosing these parameters for a given estuary.

To demonstrate the predictive capability of the mathematical model the computed results are compared with available data from dye

test experiments in the James River Model at the U.S. Army Corps of Engineers Waterways Experiment Station and in Cork Harbour, Ireland. Cork Harbour also provides a practical application of the model to investigate the benefits of alternate waste disposal schemes near the ocean boundary.

CHAPTER II

THEORETICAL CONSIDERATIONS

2.1 Governing Equations and Assumptions

The assumption of one-dimensionality limits the results of a mathematical model to quantities which are spatial averages over a channel cross-section. Thus, a mean velocity is computed by dividing the tidal discharge by the cross-sectional area, and pollutant discharged at a certain location is assumed to be immediately and completely mixed across the cross-section. Immediate and complete mixing near pollutant discharges may be a reasonable assumption if the pollutant is discharged through a diffuser stretched across the channel; however, it may not be reasonable if the discharge is through an outfall pipe near the shore. Similarly, the mean tidal discharge velocity neglects the cross-sectional velocity variations which range from small values near the sides and bottom to large values in the heart of the channel. Once a cloud of pollutant is present in the channel it will be advected downstream at the mean discharge velocity, but it will be spread out as pollutant in a high velocity region moves ahead and pollutant in a low velocity region lags behind. This process is known as longitudinal dispersion, and based on observation, it is idealized as a pseudo-diffusive process.

2.1.1 One-Dimensional Conservation of Mass Equation

The basic equation for water quality simulation is a conservation of mass equation which includes the transport processes of advection and dispersion, and reaction processes whereby mass is added to or removed from the system.

Several investigators, including Okubo (1964) and Holley and Harleman (1965), have derived the one-dimensional conservation of mass equation rigorously. Only the result will be stated here in its most general form:

$$\frac{\partial}{\partial t} (Ac) + \frac{\partial}{\partial x} (Qc) = \frac{\partial}{\partial x} (AE \frac{\partial c}{\partial x}) + \left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \quad (2.1)$$

where

c = concentration of constituent

A = channel cross-sectional area

Q = tidal discharge

E = longitudinal dispersion coefficient in tidal time

ρ = density of water

r_i = time rate of internal addition of mass per unit volume by generation of substance within the fluid

r_e = time rate of external addition of mass per unit volume by movement across the boundaries of the fluid

The reaction processes represented by r_i and r_e will vary depending on the water quality constituent being considered. For a conservative substance such as salinity, they will both be zero. Bio-chemical oxygen demand (BOD), however, is non-conservative, and its internal removal within the water mass is often described in terms of a so-called first-order reaction where $r_i = -Kc$. The first order reaction coefficient K is expressed typically in units of day^{-1} . A source term of the external type would be replenishment of dissolved oxygen (DO) by transfer across the free surface from the atmosphere.

If a given constituent is part of a set of constituents which interact with each other, a conservation of mass equation is written for each one. For the four constituents considered in the present study, salinity, temperature, BOD, and DO, the conservation of mass equations are:

$$\text{Salinity: } \frac{\partial}{\partial t} (As) + \frac{\partial}{\partial x} (Qs) = \frac{\partial}{\partial x} (AE \frac{\partial s}{\partial x}) \quad (2.2)$$

$$\text{Temperature: } \frac{\partial}{\partial t} (AT) + \frac{\partial}{\partial x} (QT) = \frac{\partial}{\partial x} (AE \frac{\partial T}{\partial x}) - K_T A (T - T_e) \quad (2.3)$$

$$\text{BOD: } \frac{\partial}{\partial t} (AL) + \frac{\partial}{\partial x} (QL) = \frac{\partial}{\partial x} (AE \frac{\partial L}{\partial x}) - K_1 AL \quad (2.4)$$

$$\text{DO: } \frac{\partial}{\partial t} (AC) + \frac{\partial}{\partial x} (QC) = \frac{\partial}{\partial x} (AE \frac{\partial C}{\partial x}) - K_1 AL + K_2 A (C_s - C) \quad (2.5)$$

where

s = salinity concentration

T = temperature

T_e = equilibrium temperature

L = BOD concentration

C = DO concentration

C_s = saturation concentration of DO

K_T = temperature decay coefficient

K_1 = BOD decay coefficient

K_2 = reaeration coefficient

BOD and DO are influenced by the salinity and temperature distributions

in addition to the coupling through the decay term - K_1AL . In the salinity intrusion region, the velocity variations across the channel cross-section are much larger than those in the fresh-water tidal region, thereby increasing the effects of longitudinal dispersion by as much as one or two orders of magnitude. Thatcher and Harleman (1972) have related the longitudinal dispersion coefficient E to the local salinity gradient, both in space and time, and have found good success in matching computed salinity distributions with field data. Salinity and temperature also affect the reaction process of BOD and DO. The BOD decay coefficient K_1 is dependent on temperature, and C_s , the DO saturation concentration, is dependent on the salinity content of the water.

The most important term in the conservation of mass equation is the advective term which describes longitudinal movement of a water quality constituent by the tidal discharge. The most direct method of determining the tidal discharge is by current measurements in the field. However, such data is rarely available and it is usually necessary to generate the discharges mathematically. One technique for doing so is known as the method of cubature, which involves an integration of the continuity equation for water.

2.1.2 Continuity Equation for Water

The continuity equation and the longitudinal momentum equation which follows are sometimes known as the St. Venant Equations. They describe the process of long wave propagation in open channels and constitute mathematical expressions for the conservation of mass and momentum. Derivations of the equations have been given by a number of authors, including Gilcrest (1958), Lai (1965), and Harleman and

Lee (1969). The result for the continuity equation is:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_L \quad (2.6)$$

where

q_L = lateral inflow per unit length of the channel.

If it is assumed that the transverse water surface is horizontal, which implies that channel curvature and Coriolis effects are negligible, the area term may be rewritten as:

$$\frac{\partial A}{\partial t} = B \frac{\partial z}{\partial t} \quad (2.7)$$

where

B = channel topwidth

z = water surface elevation with respect to an arbitrary horizontal datum

After substitution, the continuity equation becomes:

$$B \frac{\partial z}{\partial t} + \frac{\partial Q}{\partial x} = q_L \quad (2.8)$$

In many estuaries, the tide ranges, phase lags, and fresh water inflows are reasonably well-known or they can be obtained at moderate expense by a tide gage survey. Integration of the continuity equation provides a simple technique to convert this information into discharges along the axis of the estuary.

$$Q(x) = \int_0^x q_L dx - \int_0^x B \frac{\partial z}{\partial t} dx \quad (2.9)$$

This procedure is known as the method of cubature. The integrals on the

right-hand side of Equation (2.9) may be evaluated explicitly once functional forms are assumed for the integrands. As an example, consider an estuary where the only lateral inflow is fresh water inflow at the head of tide:

$$q_L = Q_f \delta(x - 0) \quad (2.10)$$

where

$\delta(x - 0)$ is the Dirac delta functions.

The topwidth as a function of distance can be evaluated from coast charts and maps:

$$B = B(x) \quad (2.11)$$

The surface elevation may be approximated as a sinusoid with prescribed variations in amplitude and phase:

$$z(x, t) = z_0(x) + \frac{a(x)}{2} \cos \sigma\{t - \tau(x)\} \quad (2.12)$$

where

$z_0(x)$ = local mean water surface elevation

$a(x)$ = local tide range

$\sigma = \frac{2\pi}{T}$ = angular frequency

T = tidal period

$\tau(x)$ = local phase lag of tidal elevation

Then the discharges may be determined by explicit evaluation of the integral expression:

$$Q_x = Q_f + \frac{\sigma}{2} \int_0^x B(x) \cdot a(x) \sin \sigma\{t - \tau(x)\} dx \quad (2.13)$$

An alternative to analytical integration of the continuity equation is a numerical solution technique for the discharge which was proposed by Wicker (1955).

It should be noted that the method of cubature is not predictive in that it depends on known tidal characteristics of the estuary. If the hydrography of the estuary were to be changed by dikes, filling, channel dredging, etc., the tidal characteristics would change also. The only way to predict the new tidal response is to execute a combined solution of the continuity equation and the longitudinal momentum equation.

2.1.3 Longitudinal Momentum Equation Including Density Effects

This equation describes the longitudinal transport of momentum, and it can be expressed in a form similar to the conservation of mass equation:

$$\frac{\partial}{\partial t} (AU) + \frac{\partial}{\partial x} (QU) = - Ag \left(\frac{\partial z}{\partial x} + \frac{U|U|}{C_z^2 R_h} \right) \quad (2.14)$$

where

U = cross-sectional average velocity = Q/A

g = acceleration of gravity

C_z = Chezy coefficient

R_h = hydraulic radius

In deriving this form of the momentum equation it is assumed that pressure over the depth of the channel is hydrostatic, i.e., vertical accelerations are neglected and the density of the fluid is assumed to be homogeneous. Also, it is assumed that momentum dissipation through

the effects of boundary friction and turbulence may be described by an empirical formula such as the Chezy equation. For computations in estuaries, the assumption of homogeneous fluid density is not strictly correct in the salinity intrusion region near the ocean. Thatcher and Harleman (1972) and Fisher, Nava and Cross (1970) have included an extra term in the momentum equation to account for the effects of longitudinal density gradients:

$$g \frac{A d_c}{\rho} \frac{\partial \rho}{\partial x}$$

where

ρ = fluid density

d_c = depth to the centroid of the channel cross-section

To place the momentum equation in a convenient form for numerical solution, two more manipulations are useful. In the form of Equation (2.14), derivatives of both velocity and discharge will appear. Since most numerical solutions are in terms of water surface elevation and discharge, the velocity derivative may be eliminated through the relationship:

$$\frac{\partial Q}{\partial x} = U \frac{\partial A}{\partial x} + A \frac{\partial U}{\partial x} \quad (2.15a)$$

or

$$Q \frac{\partial U}{\partial x} = U \frac{\partial Q}{\partial x} - U^2 \frac{\partial A}{\partial x} \quad (2.15b)$$

Also, non-prismatic channel effects may be included with the following representation of the area derivative:

$$\frac{\partial}{\partial x} \{A(x, z(x, t))\} = \left. \frac{\partial A}{\partial x} \right|_{z=\text{const}} + \frac{\partial A}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial A^z}{\partial x} + B \frac{\partial z}{\partial x} \quad (2.16)$$

With the appropriate additions and substitutions, Equation (2.14) may be written in the form:

$$\frac{\partial Q}{\partial t} + 2U \frac{\partial Q}{\partial x} = - Ag \{ (1 - IF^2) \frac{\partial z}{\partial x} - \frac{IF^2}{B} \frac{\partial A^z}{\partial x} + \frac{U|U|}{C_z^2 R_h} + \frac{d}{\rho} \frac{\partial \rho}{\partial x} \} \quad (2.17)$$

where

$$IF = \frac{U}{c}$$

$$c = \sqrt{g \frac{A}{B}} = \text{wave celerity}$$

One further refinement that can be introduced is the notion of the so-called conveyance or core area. This is a device for recognizing that the main channels of an estuary are often flanked by side channels and embayments. These do not contribute to the longitudinal transport of momentum by currents in the main channels; however, they do store part of the water in the tidal wave as it passes. To reproduce these physical effects in the mathematical model, the cross-sectional area A in the longitudinal momentum equation is assigned the core area or conveyance area of the main channel to which the tidal discharge is confined.

$$A \rightarrow A_{\text{core}} \quad (2.18)$$

The topwidth B which appears in the continuity equation must properly reproduce the surface storage area in the main channel, the side channels, and the embayments. Therefore:

$$B \rightarrow B_{\text{core}} + B_{\text{storage}} \quad (2.19)$$

Thatcher and Harleman (1972) describe the procedure for schematizing an estuary in this manner. Their discussion will not be repeated, but one important point will be emphasized. The cross-sectional area used in the conservation of mass equation should not be the core area, but a total area including the main channel and embayments. In this way, the correct volume of the estuary for mixing of pollutant will be reproduced.

2.2 Review of Existing Water Quality Models

In recent years, a large number of water quality models have been proposed in the literature. Only those which bear directly on the one-dimensional network problem or contain features useful to its formulation will be reviewed here. An excellent review of many models which have found wide use in engineering practice is contained in TRACOR (1971). Therefore, discussions of models which are contained in this reference will be limited to their basic formulation and important operational features.

As a point of departure, some investigators choose a modified form of the conservation of mass equation. The modified form is obtained by splitting the storage and advective terms in Equation (2.1) and substituting the continuity equation for water:

$$A \frac{\partial c}{\partial t} + \underbrace{C \left(\frac{\partial A}{\partial t} + \frac{\partial \phi}{\partial x} \right)}_{q_L} + Q \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left(AE \frac{\partial c}{\partial x} \right) + \left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \quad (2.20)$$

Dividing through by A and moving the dilution term to the right-hand side:

$$\frac{\partial c}{\partial t} + \frac{Q}{A} \frac{\partial c}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(AE \frac{\partial c}{\partial x} \right) - \frac{q_L c}{A} + \left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} \quad (2.21)$$

If there are no sources, sinks, or lateral inflow, and if the quantities Q, A, and B are assumed to be constant both Equation (2.1) and Equation (2.21) reduce to the classical convective-diffusion equation:

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} = E \frac{\partial^2 c}{\partial x^2} \quad (2.22)$$

2.2.1 Non-Tidal Advective Models

Prior to the era of widespread access to high-speed computers, unsteady tidal motion in the advective term of the conservation of mass equation made evaluation of pollutant distributions extremely difficult. Recognizing that net seaward movement of pollutant is controlled primarily by fresh water throughflow, investigators proposed models which neglected the tidal motion and yielded results on a time scale of tidal periods. Advection was assumed to be due to fresh water throughflow only, and two approaches developed within the context of this assumption.

Arons and Stommel (1951) and Stommel (1953) proposed a model where each term in the conservation of mass equation is averaged over a tidal period. Neglecting lateral inflows and source terms, Equation (2.21) in time-averaged form becomes

$$\frac{\partial \bar{c}}{\partial t} + U_f \frac{\partial \bar{c}}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(\bar{AE} \frac{\partial \bar{c}}{\partial x} \right) \quad (2.23)$$

where

$\bar{c}$ = concentration averaged over a tidal period.

U_f = time averaged mean cross-sectional velocity due to fresh-water throughflow.

$\bar{A}$ = cross-sectional area time averaged over a period.

$\bar{E}$ = longitudinal dispersion coefficient time-averaged over a period.

O'Connor (1965) followed a somewhat different approach and proposed a model which eliminated the tidal motion by considering pollutant distributions only at slack tide conditions. The effect of the model is to take a "snap-shot" of the pollutant distribution once every tidal period rather than to consider time-averages over the period. Slack tide conditions were probably chosen because these were times when data on parameters such as salinity were available. The form of the conservation of mass equation considered by O'Connor is similar to that of Equation (2.23):

$$\frac{\partial c_s}{\partial t} + U_f \frac{\partial c_s}{\partial x} = \frac{1}{A_s} \frac{\partial}{\partial x} (A_s E_s \frac{\partial c_s}{\partial x}) \quad (2.24)$$

where

c_s = slack tide concentration

A_s = slack tide area (not a function of time)

E_s = slack tide dispersion coefficient (not a function of time)

O'Connor obtained analytic solutions of Equation (2.24) for cases where E_s is constant and the area A_s is either constant or a linear, quadratic, or exponential function of x . The basic solutions are for an instantaneous injection of mass, and the solutions for continuous injection

follow as an integration of instantaneous injections.

To consider the variation of water quality parameters over a long term such as seasons in an estuary of complex geometry, Thomann (1963) developed a non-tidal advective model based on numerical solution techniques. No attempt is made to solve the conservation of mass equation directly. Instead the estuary is divided into finite segments, and expressions are written for advective and diffusive transfers between segments. Thus, the model attempts to simulate discrete mass transfer processes rather than solve, in approximate form, the continuous process represented by the conservation of mass equation. The techniques of Thomann, as well as those of O'Connor are discussed in Chapter III of TRACOR (1971).

Chapter II of TRACOR (1971) contains a thorough discussion of non-tidal advective models by Harleman. As pointed out by Harleman, the non-tidal advective models are forced to exaggerate the effects of dispersion in order to account for movement of mass by tidal motion within the tidal period. This may be seen by considering movement of mass upstream of an injection point. In tidal time, flood velocities will advect mass upstream and the interaction of turbulence generated by the tidal motion with spatial velocity variations across the cross-section will disperse it. After several tidal cycles, a concentration distribution over a distance of about one tidal excursion will be created by the combined mechanism of advection and dispersion. The non-tidal advective models have no upstream advection mechanism; therefore, their dispersion coefficients must be increased by one or two orders of magnitude to achieve an upstream concentration distribution

which is a poor approximation of the actual distribution. Because there is no real physical mechanism on which to base theoretical predictions of these dispersion coefficients; they must be evaluated by expensive dye tests in the field.

The mechanism of upstream mass transport is especially important when considering the problem of salinity intrusion. Thatcher and Harleman (1972) review several applications of the non-tidal advective approach to modeling salinity intrusion. The dispersion coefficients are usually descriptive rather than predictive. If the tidal characteristics of the estuary were changed, there would be no theoretical way to predict the new dispersion coefficients. A further descriptive feature involves salinities at the ocean boundary. These have to be specified from field data or statistical predictions based on such data.

The ocean boundary condition requirement and the averaging period of the non-tidal advective models prevent them from considering waste disposal schemes whereby pollutant is injected near the ocean boundary during short periods on ebb tide only. The notion is that most of the pollutant from a given injection will be carried out to sea, dispersed, and transported away by longshore currents. Such schemes may be economically attractive if the cost of detention facilities is much less than the cost of new treatment facilities.

2.2.2 FWQA Dynamic Estuary Model

The FWQA Model is often referenced in the literature as the Orlob Model, after Dr. Gerald T. Orlob, who did the development work. It is a versatile model and it has been applied to numerous problems in engineering practice. The description "dynamic" refers to the fact that

the model includes the effects of tidal motion rather than neglecting them, as in the non-tidal advective models.

In formulating the model, the primary intent was to provide capability for handling a large, complex network of channels such as the Sacramento-San Joaquin Delta in California. The network was conceptualized as a series of uniform channels connected to junctions, or nodes. The junctions act as reservoirs which store all the mass in the system, and the channels serve as conduits for flows between junctions.

The unsteady hydrodynamics of the physical system are defined by the continuity and longitudinal momentum equation for constant area channels in the form:

$$\frac{\partial z}{\partial t} = - \frac{1}{B} \frac{\partial Q}{\partial x} + q_L \quad (2.25)$$

$$\frac{\partial U}{\partial t} = - U \frac{\partial U}{\partial x} - k |U|U - g \frac{\partial z}{\partial x} \quad (2.26)$$

In addition to the assumptions listed in section 2.1.3, Equation (2.26) assumes that the channels are prismatic and level. Although these equations describe the continuous process of unsteady flow in open channels, they are adapted to describe tidal flows between discrete control volumes represented by the junctions. A continuity equation is written for each junction in the form:

$$\frac{\Delta z_j}{\Delta t} = \frac{\Sigma Q_j}{A_j^*} \quad (2.27)$$

where

ΣQ_j = summation of flows into the junction both from channels and lateral inflows

A_j^* = surface area of the junction

Then a discretized momentum equation is written to define the flows in each channel:

$$\frac{\Delta U_i}{\Delta t} = - U_i \frac{\Delta U_i}{\ell_i} - k |U_i| U_i - g \frac{\Delta z_i}{\ell_i} \quad (2.28)$$

where

ℓ_i = length of channel i

ΔU_i = velocity change across channel i

Δz_i = water surface elevation i

U_i = velocity in channel i

Inasmuch as a single velocity U_i is calculated for each channel, there is no way to evaluate the change ΔU_i . Therefore, a discretized version of Equation (2.25) is used to eliminate ΔU_i . After this manipulation, a modified Runge-Kutta procedure is used to solve for the channel velocities U_i and the junction water surface elevation z_j .

The water quality model is superimposed on the hydraulic model, using the same channels and junctions. Conservation of mass throughout the system is achieved by writing a discrete conservation of mass equation for each junction. Included are additions by mass transported through the channels, additions or removals through reaction processes,

and import or export by waste discharge or diversion. In the version of the model documented by Feigner and Harris (1970), the reaction processes are assumed to follow first-order kinetics and mass transport through the channels is by two mechanisms:

Mass Transport by Advection

$$\Delta M_a = A_i U_i c^* \Delta t \quad (2.29)$$

where

ΔM_a = the mass advected through the channel from the upstream junction to the downstream junction during the time step Δt .

A_i = cross-sectional area of channel i during the time step Δt .

c^* = a representative concentration of the water in the channel.

Mass Transport by Eddy Diffusion

$$\Delta M_d = K_d A_i \frac{\Delta c_i}{\ell_i} \Delta t \quad (2.30)$$

where

ΔM_d = the mass diffused along channel i from the junction of higher concentration to the junction of lower concentration.

K_d = eddy diffusion coefficient in channel i during the time step Δt .

Δc_i = concentration difference across channel i .

It should be noted that the eddy diffusion coefficient does not include

the effects of longitudinal dispersion. Instead, it is intended that these effects be contained in the effects of numerical dispersion.

Numerical dispersion results when there is a significant concentration gradient along the channel, and a given water parcel moves only a portion of the channel length. Mathematically, a given mass of substance is transferred from the upstream junction to the downstream junction. Physically this may not occur during one time step. The representative concentration is an attempt to approximate the correct amount of mass as closely as possible. A number of expressions for c^* have been tried, and one which gave reasonable results in the California study is the so-called quarter-point formula:

$$c^* = \frac{3c_i + c_j}{4} \quad (2.31)$$

where

c_i = concentration at upstream junction i

c_j = concentration at downstream junction j

In a water quality study of the Potomac estuary, Clark and Feigner (1972) found that the quarter point formula did not give good results and used a third-point formula instead. Feigner and Harris note that no single criterion is available to define the optimum combination of time step, network scale, eddy diffusion coefficient, and method of advective transport. Therefore, the best representative concentration for a particular application must be determined by matching field data. If a criterion were available, it would have to be compatible with stability requirements for the hydraulic model which uses the same network of channels and junctions.

A disadvantage of the FWQA Model is that the user must specify the ocean boundary concentration of a particular water quality parameter over the entire tidal cycle. This requirement is especially difficult when dealing with water quality phenomena near the ocean boundary such as salinity intrusion and waste disposal schemes which utilize the benefits of tidal flushing. In essence, the user must know the final results before he starts. To circumvent the problem, Feigner and Harris recommend that users locate the ocean boundary as far as possible from the region of concern and try to specify the boundary condition in such a way that it not significantly bias the numerical results. In practice, this may not always be possible.

Operation of the model is straightforward. At a given time step, the mass transfers due to advection and diffusion are determined for each channel. These transfers are summed at each junction and a new mass in the junction is computed. If the substance is non-conservative, a correction is made to account for gain or loss by reaction processes. Additional gains or losses by inflows or withdrawals are taken into account and then new concentrations for the junctions are computed.

Before a new cycle through the computational procedure is begun, a check is made for negative concentrations in the junctions. If a concentration is negative, it is reset to zero. This is incorrect in that mass is being added to the system artificially to offset the negative concentrations. One possible situation where negative concentrations might occur is in the modeling of dissolved oxygen under nearly anaerobic conditions. If the BOD decay term - K_1AL in Equation

(2.5) overshadows the reaeration term at zero DO, K_2AC_s , the mathematical results will be negative concentrations. Physically, the situation is unrealizable because BOD decay at zero DO will be limited to the amount of oxygen transmitted into the system by reaeration. Then the reaeration and decay term will cancel and water will be transported at zero DO until reaeration exceeds decay and DO begins to rise. One way to deal with the situation properly in the computer is to require that $|K_1AL| \leq |K_2AC_s|$ where $C \approx 0$.

Negative concentrations may also be associated with the presence of steep concentration gradients which the numerical solution finds difficult to reproduce. The numerical solution oscillates about the true solution, and it may go negative if the true solution is near zero. Although this is mathematically and physically acceptable, some people find any negative concentrations bothersome. The appropriate remedy is refinement of the network scale, the time step, or both, in order to achieve better resolution of the gradient.

2.2.3 Lagrangian Method of H.B. Fischer

To minimize the problems of numerical dispersion in water quality models based on Eulerian or control volume concepts, Fischer (1969) devised a network model using a Lagrangian formulation. The channels of the network are divided into segments of uniform depth and width, and the water within each segment is sub-divided into volume elements, each having its own concentration.

The computations proceed in tidal time in sequences of three steps, a convective step, a diffusive step, and a decay step. In the convective

step, the volume elements in a segment are moved downstream at the mean tidal velocity in that segment. The velocity must be supplied from either field measurements or mathematical computations. In a later version of the model, Fischer (1970) calculates the tidal hydraulics using the method of characteristics on a fixed grid, as developed by Lai (1967). The outflow from a segment is made up of that portion of the volume elements which are convected beyond the downstream end of the segment. The concentration of the outflow is the mixed concentration of the participating volume elements. If two or more segments flow into a third, the inflow is the mixed concentration of the outflows. Some longitudinal dispersion could occur in these mixing computations, but Fischer does not consider it too significant.

Following the convective step is a diffusive step, wherein mass transfers are made between adjacent elements in a volume segment to simulate the dispersion process. Diffusive transfers are not made across the ends of channels in order to keep the computer programming simple. Noting that adjacent elements can have different lengths, Fischer defines the diffusive mass transfer as:

$$\Delta M_d = {}^0E \frac{T}{l_s} \frac{B}{l_s} (c_l - c_s) l_s \quad (2.32)$$

where

ΔM_d = mass per unit depth and width (note that depth and width are identical for all elements in a segment).

${}^0E$ = dimensionless mass transfer coefficient supplied by the user
(Fischer recommends a value of about 0.2).

T = distance travelled by the shorter element during the convective step.

B = channel width.

ℓ_s = length of the shorter element.

c_s = concentration of the shorter element.

c_ℓ = concentration of the larger element.

The factors $\frac{T}{\ell_s}$ and $\frac{B}{\ell_s}$ are adjustments to the mass transfer coefficient ^oE to account for the effects on dispersion of distance travelled by the shorter element and its length to width ratio. For numerical stability, the product $^oE \frac{T}{\ell_s} \frac{B}{\ell_s}$ must always be less than 0.5.

After the diffusive step is completed, the concentrations in the volume elements are reduced by a fixed percentage to simulate a first order decay process. Then the three-step sequence is cycled through once more. The user need not specify an ocean boundary concentration during ebb tide, as in the FWQA Model. Volume segments are simply carried out to sea. On flood tide, the concentration of incoming volume segments could be specified at known values to reflect the return of waste.

Operationally, the model would seem to involve some rather complex bookkeeping procedures, even though some simplifications were made. At present, it is limited to tree-like networks, and Fischer notes that some trouble was experienced which was due to the generation of many short volume elements near the ends of terminal segments. These short elements were combined into larger ones. Treatment of the diffusive step is highly empirical, and the user would have to adjust the mass

transfer coefficient arbitrarily by matching field data.

2.2.4 Tidal Time Models of Lee and Harleman and of Thatcher and Harleman

Both the FWOA Model and Fischer's Model set up the water quality computations in terms of a series of control volumes for which the mass transfer and reaction processes are written. Lee and Harleman (1971) took a different approach and formulated a finite difference solution of the conservation of mass equation in a single-channel estuary. The solution includes the tidal motion and allows time and space variation of cross-sectional area, discharge, and dispersion coefficient. To drive the water quality solution, the tidal hydraulics are obtained by a finite difference solution of the continuity and momentum equations in tidal time. The finite difference scheme used to solve the conservation of mass equation is a generalization of the 6-point implicit scheme recommended by Stone and Brian (1963) for solving the convective diffusion equation. Figure 2.1 shows the computational molecule and the weighting factors for the Stone and Brian scheme.

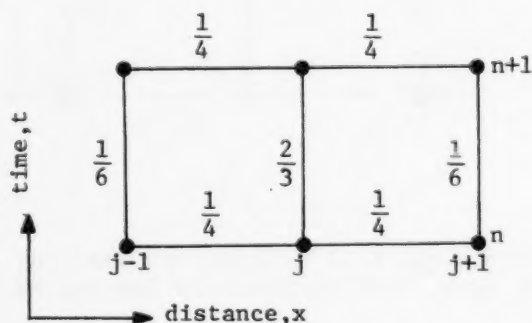


Figure 2.1 Computational Molecule for the Stone and Brian Scheme

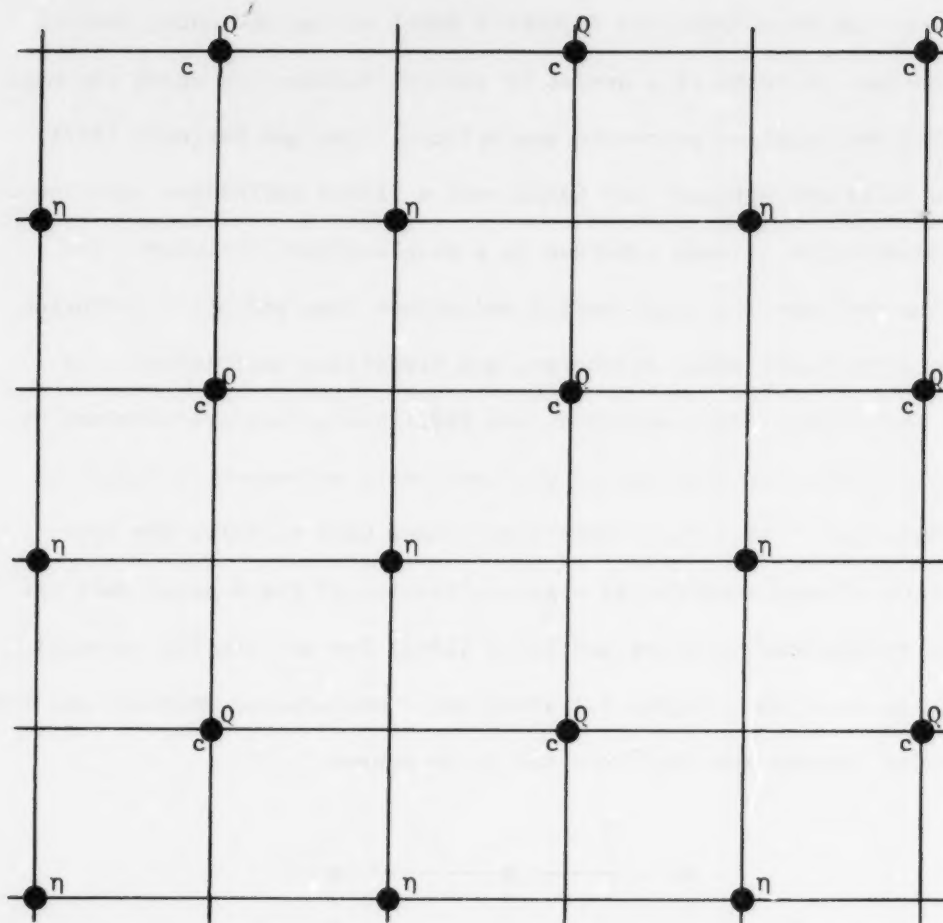


Figure 2.2 Computational Grid in Space and Time for the Tidal Hydraulics and Water Quality Models of Lee and Harleman

The computational molecule for the water quality model is superimposed on the computational grid for the tidal hydraulics model by calculating concentrations at discharge mesh points, as shown in Figure 2.2. The grid is staggered in space and time, and the finite difference scheme which uses this grid is sometimes called the "leap-frog method". Formulating the scheme in this way yields a solution procedure which is numerically accurate and computationally efficient.

In applying the water quality model to some sample problems, Lee and Harleman found that the solution tended to oscillate markedly in the vicinity of steep concentration gradients. The oscillations could be diminished if Δx and/or Δt were reduced, but this imposes a penalty in longer computer time. Since finite difference solutions require a constant mesh spacing Δx , one cannot compress the mesh where concentration profiles are steep and stretch it where the profiles are flat. Lee and Harleman found that the oscillations could be smoothed out by using a technique called "two-step averaging". This was done on output only, so that it had no internal effect on the solution. However, the resulting profile did not necessarily agree with the correct solution, for the oscillations are symptomatic of the model's inability to reproduce the correct, smooth solution.

Thatcher and Harleman (1972) adapted the Lee and Harleman model to study the problem of salinity intrusion in a single-channel estuary. To describe the increased effects of longitudinal dispersion in the salinity intrusion region, the local dispersion coefficient was expressed as:

$$E(x,t) = K \left| \frac{\partial s^0}{\partial x} \right| + E_T \quad (2.33)$$

where

$$\frac{s^0}{s} = s/s_o$$

s = salinity

s_o = ocean salinity

$$\frac{x^0}{x} = x/L$$

L = length of the estuary

K = a parameter related to the degree of stratification in the estuary

E_T = Taylor dispersion coefficient

$$= 77nUR_h^{5/6}$$

n = Manning resistance coefficient

Solution oscillations were not a great problem in this application because the increased dispersion stretches the salinity profile and makes the gradients less steep. The model has been very successful in predicting the transient behavior of salinity distributions both in prototype estuaries and hydraulic model studies.

Thatcher and Harleman also give a detailed discussion of the considerations which arise in formulating boundary conditions in finite difference models. Any finite difference scheme takes the governing partial differential equation and discretizes it in terms of mesh points in the interior of the solution domain. If the solution variable, say concentration, is specified at the boundary mesh points, there are enough

equations in enough unknowns to evaluate the interior mesh point concentrations in a straightforward manner. However, the boundary concentration is not always specified, as is the case at the ocean boundary of an estuary on ebb tide. Then it is necessary to have another equation for the boundary concentration which includes a statement of the boundary condition which is mathematically required for a unique solution of the problem. In formulating this equation, care must be taken to insure that conservation of mass properties of the solution as a whole are preserved.

On ebb tide, the ocean boundary is merely a stopping point for the computations; it does not constrain the seaward movement of mass. Hence, there is no clear-cut mathematical statement of a boundary condition. Both Lee and Harleman and Thatcher and Harleman get around this problem by writing a mass balance over the segment adjacent to the boundary. Contained within this mass balance is the assumption that the dispersive flux over the boundary segment remains constant.

It is not clear that this type of boundary condition statement is strictly correct in a mathematically rigorous sense; however, it seems to work computationally. The likely reason for this is that the ocean boundary concentration is dominated by advection from upstream on ebb tide. Assumptions regarding the dispersive flux probably have very little effect on the solution.

2.2.5 Finite Element Approaches

The finite element method, like the finite difference method, is directed towards obtaining a numerical solution of a partial differential

equation such as the conservation of mass equation (2.1). However, the points of departure of the two methods are quite different. In the finite difference method, the solution domain is discretized into a computational mesh as shown in Figure 2.3.

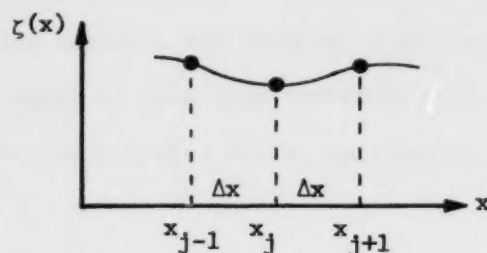


Figure 2.3 Definition Sketch for Finite Difference Method

The derivatives in the partial differential equation are approximated as simple differences

$$\left. \frac{\partial \zeta}{\partial x} \right|_{x=x_j} \approx \frac{\zeta_{j+1} - \zeta_{j-1}}{2\Delta x} \quad (2.34)$$

where ζ_j is an approximation of the exact continuous solution at mesh point j . Usually the mesh spacing Δx is held constant to permit the use of higher order difference approximations. With all the derivatives replaced by differences, there results a set of equations for all the $\bar{\zeta}_j$.

Figure 2.4 shows a similar mesh for the finite element method.

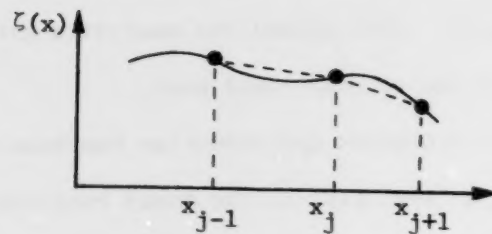


Figure 2.4 Definition Sketch for Finite Element Method

Here, the solution itself, rather than its derivatives, is approximated by a piecewise continuous function such as a series of straight lines.

The piecewise continuous approximation can be expressed as:

$$\zeta(x,t) = \sum_{j=1}^M \phi_j(x) \zeta_j(t)$$

where the $\phi_j(x)$ are interpolating functions and $\zeta_j(t)$ is a time-varying approximation of the exact continuous solution at mesh point j . An example of $\phi_j(x)$ for the straight line approximation is given in Figure 2.5. (See Zienkiewicz and Cheung (1967)).

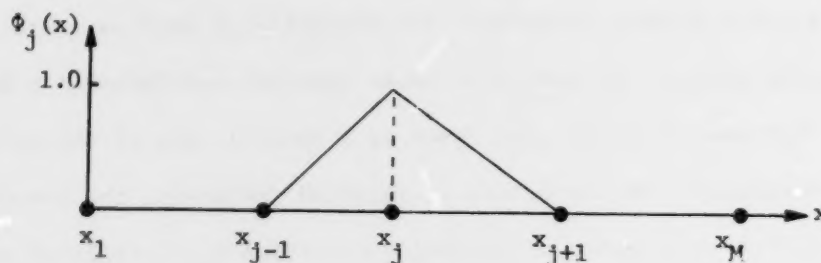


Figure 2.5 Interpolating Function $\phi_j(x)$ for a Piecewise Linear Approximation

It may be noted from Figure 2.4 and Figure 2.5 that the spacings between mesh points can be variable. This allows the analyst a great deal of flexibility in setting up the computational mesh.

After the piecewise continuous approximation has been written, it must be adjusted to give a "best fit" to the exact continuous solution. Two techniques are commonly used to perform the adjustment, the method of weighted residuals and an approach based on the calculus of variations.

2.2.5a The Method of Weighted Residuals

When the piecewise continuous approximation is substituted into the partial differential equation, a residual will exist because the exact, continuous solution is not matched. The residual may be defined as:

$$R = \langle L(\zeta) \rangle - L(\zeta) \quad (2.36)$$

where

$L(\zeta)$ = the partial differential equation

$\langle L(\zeta) \rangle$ = the discretized form of the partial differential equation.

To obtain a "best fit" between the piecewise continuous approximation and the exact, continuous solution, the residual R must be minimized. Crandall (1956) discusses several techniques for minimizing R such as collocation, the subdomain method, the method of least squares, and Galerkin's Method. He shows that each of these techniques is a special case of the method of weighted residuals. In the method of weighted residuals, the residual R is multiplied by a series of weighting functions w_i , integrated over the length of the solution domain L and set to zero.

$$\int_L w_i R dx = 0, \quad i = 1, \dots, M \quad (2.37)$$

In principle, there are now M equations for M unknown solution variables at the mesh points.

Price, Cavendish, and Varga (1968) applied the method of weighted residuals in the form of Galerkin's Method to the convective diffusion equation. In Galerkin's Method the weighting functions w_i are taken as the interpolating functions ϕ_i . Price, et.al., compared the results of the weighted residuals technique with results obtained by using standard finite difference techniques and a technique based on the method of characteristics. They found that the method of weighted residuals yielded higher numerical accuracies and consumed less computer time.

2.2.5b Variational Techniques

Variational techniques have been applied extensively in the fields of structures, solid mechanics, and flow in porous media. In these fields, problems are often defined by elliptic partial differential equations such as Laplace's Equation. For these problems, it is often possible to formulate a variational parameter such as the strain energy or complementary strain energy in solid mechanics. The piecewise continuous approximation of the solution is entered in the expression for the variational parameter, and the calculus of variations is applied to adjust the approximation to a "best fit".

Guymon (1970) developed a variational principle for the one dimensional conservation of mass equation in the form:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(AE \frac{\partial c}{\partial x} \right) \quad (2.38)$$

The main advantage of the variational principle is that it yields a set of symmetric matrices, whereas the matrices obtained from the method of weighted residuals are non-symmetric. Symmetric matrices are advantageous in higher dimensions where computer storage can be a problem. In one-dimensional problems, however, the matrices are tridiagonal, so that the savings in storage and computer time are not too significant.

There is a subtle problem associated with the form of the conservation of mass equation chosen by Guymon. This is analogous to Equation (2.21) which was obtained from Equation (2.1) by substituting the continuity equation, Equation (2.6). Leendertse (1971) has indicated that numerical solutions based on the modified conservation of mass equation with variable coefficients may not conserve mass. The reason for this may be observed by considering the mechanics of deriving Equation (2.1). Equation (2.1) may be derived by writing a mass balance for a finite volume of the channel, $A\Delta x$, over a short time Δt and taking the expression to the limit. Intuitively, a numerical scheme based on Equation (2.1) should conserve mass, since it may be thought of as simply backing away from the limit to consider finite control volumes once again. At the limit however, the derivatives of Equation (2.1) may be expanded, and certain terms may be eliminated with the continuity equation to obtain Equation (2.21). As Leendertse points out, this is an equation for the concentration distribution at the limit and does not in itself represent a mass balance. Therefore, it is not surprising that a numerical solution based on Equation (2.21) may not conserve mass. Guymon does not discuss this problem, as he deals only with constant area, velocity, and dispersion coefficients, for which Equation (2.1) reduces directly to Equation (2.22), the convective diffusion equation. -58-

2.3 Formulation of a New Approach to the Network Problems

2.3.1 Areas of Application

The geometry of an estuary can be very complex, often consisting of channels and embayments connected in some arbitrary manner. Building a practical mathematical model for such a general estuary is an extremely difficult task; therefore, assumptions must be made to reduce the complexity of the problem. The assumption of one-dimensionality considerably reduces computational requirements, while the network formulation preserves the ability to describe highly complex geometries.

A one-dimensional network model may be applied in a straightforward manner to the typical estuary of Figure 1.1 where flow is along the axes of well-defined channels. To describe the estuary completely, the boundaries are located at ocean entrances where the tides are known and at heads of tide where fresh water inflows are prescribed. Therefore, the computations will include both the salinity intrusion region and the fresh water tidal region of the estuary. The transport of pollutant in the salinity intrusion region will be strongly affected by increased longitudinal dispersion which is caused by salinity gradients. To reproduce these effects properly, salinity can be included as one of constituents in the mathematical model. Dispersion coefficients similar to those calculated by Thatcher and Harleman (1972) may be used to determine the salinity distribution and describe dispersive transport of other constituents as well. It should be noted that the Thatcher and Harleman coefficients are based on a correlation of certain gross normalization parameters for a single-channel estuary. Among these

are channel length, maximum salinity at the ocean end, fresh water throughflow, and maximum velocity at the ocean end. For a particular channel within the overall frame of a network, it is not obvious how these normalization parameters should be chosen. Dispersion criteria based on more localized parameters should evolve in time; however, it should be possible for the present to use the Thatcher and Harleman criteria subject to some assumptions. Channels which are side branches of a network might be considered as miniature single-channel estuaries with appropriate normalization parameters. This is the way Thatcher and Harleman treated the Potomac, which is really an arm of Chesapeake Bay. Channels which are located on a main stem of the network could be characterized by normalization parameters which are determined by the scale of the main stem. The proper form of these assumptions and the nature of their limitations must be found by case studies.

The concepts of the one-dimensional network model can be stretched to include estuaries with a certain amount of embayment. In particular, the FWQA Model has been used with some success to describe flows and movement of water quality constituents in the San Francisco Bay system. It is felt that application of one-dimensional concepts should be limited to bays which are reasonably well-channelized. The directions of flow are determined, and the effects of Coriolis force and wind shear will be less than if the bay had a broad flat bottom. This type of channelized hydrography is a feature of Cork Harbour in Ireland, which is sketched in Figure 2.6. A deepwater channel passes from the ocean through the open bay area of the Lower Harbour, past the city of

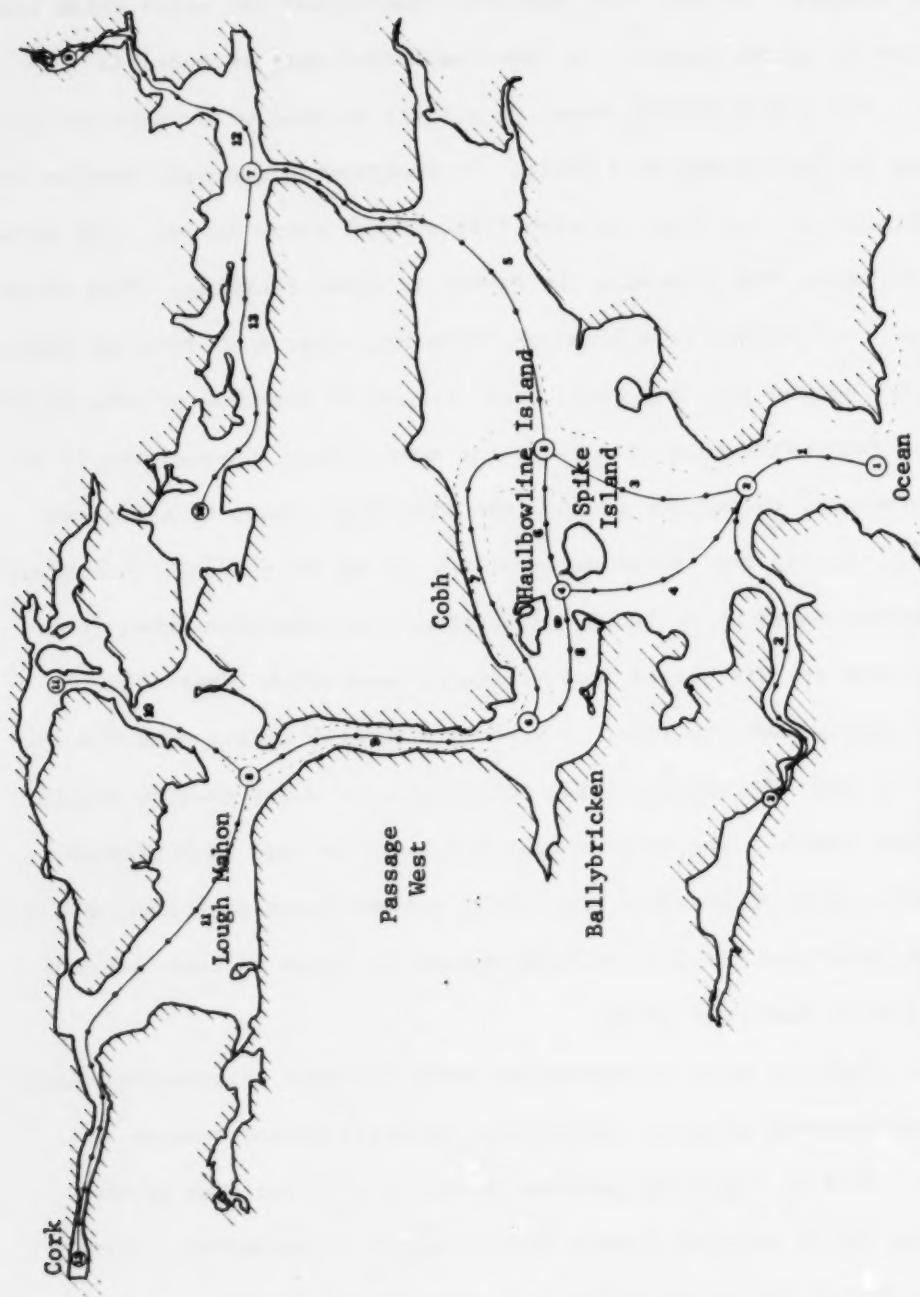


Figure 2.6 Schematic Map of Cork Harbour, Ireland

Cobh, and on to the Upper Harbour at Cork. The geometry of the system is very complex; it has open, somewhat channelized bay areas which are connected by narrow straits. A one-dimensional network model is probably the only practical means at present to deal with water quality problems in the estuary as a whole. An important hydrologic feature of Cork Harbour is that there is very little fresh water inflow. The principal mechanism for cleansing the harbor is tidal flushing. This means that waste discharged at a location where the water mass does not leave the harbor on ebb tide may cause a concentration increase to unacceptable levels. Faced with this situation, one must either increase the level of treatment of the wastes or move the discharge closer to the ocean entrance. Within the latter alternative, it may be possible to minimize the distance moved by designing an intermittent injection schedule in which wastes are discharged into the water mass which leaves the estuary during each ebb tide. A trade-off process exists with the objective of each alternative being maintenance of water quality within prescribed limits. The mathematical model can be used to determine the alternatives which yield acceptable concentration distributions, and these alternatives may then be rank-ordered in terms of cost and consistency with long-term goals.

One long-term goal in evaluating waste disposal alternatives might be the maintenance of water quality in the ocean waters outside an estuary. This is a growing problem in bodies of water such as the North Sea, which receives wastes from a number of estuaries. Interestingly, Ryther (1971) has noted that some wastes constitute a nutrient source for marine life in the ocean. Although non-toxic, organic

wastes may result in low dissolved oxygen levels when highly concentrated in estuaries, such wastes can be beneficial when they are diluted in the ocean. Therefore, productivity of the oceans might be stimulated if these wastes were not removed by treatment and were routed to the ocean in such a way that estuarine water quality is maintained.

2.3.2 Evaluation of Existing Techniques

Discussion of the water quality problem in Cork Harbour in the preceding section emphasizes one of the major deficiencies of non-tidal advective techniques in formulating a network water quality model. Within a tidal excursion of the ocean boundary, they cannot describe the removal of wastes by tidal flushing, due mainly to the time scale assumed. Also, negligible fresh water inflow in Cork Harbour means that the waters are generally near ocean salinity, especially in the Lower Harbour. Without a salinity distribution as an indicator, empirical dispersion coefficients to obtain upstream movement of pollutant would have to be evaluated by dye tests which can be expensive.

Two existing network models include the effects of tidal motion, Fischer's Model and the FWQA Model. Both of these are conceptualized in terms of control volumes. In Fischer's Model finite volumes of water are routed through the network in a sequence of convective, diffusive and decay steps. The model seems to require a considerable amount of bookkeeping which can be operationally cumbersome on the computer. The FWQA Model considers the network as a series of reservoirs, or junctions, which are connected by channels to achieve mass transfers. At the ocean boundary, the user must specify the concentration of a particular water

water quality parameter over the entire tidal cycle. For water quality phenomena near the ocean boundary, this means that the user must know the correct boundary concentrations before the computations begin in order to model the movement of mass into and out of the estuary properly.

For a mathematical model of estuarine to be predictive, it must be able to reproduce the transport processes of advection and longitudinal dispersion accurately. Longitudinal dispersion is a very complex process, resulting from the interaction of turbulent diffusion and the shear-induced velocity distribution over the channel cross-section. Its effects are important when considering water quality problems where steep concentration gradients may exist. The FWQA Model does not simulate the effects of longitudinal dispersion directly; however, it does include an eddy diffusion term to account for the observed effects of longitudinal mixing. The eddy diffusion coefficient K_d in Equation (2.30) is a function of only the scale of turbulence in the channel. Spreading effects of the cross-sectional velocity distribution are neglected. Fischer simulates longitudinal dispersion in a very simplified manner by having the user specify a fixed percentage for diffusive or dispersive mass transfer between adjacent volume elements. This percentage is then adjusted arbitrarily within the computations to account for secondary effects such as element geometry and distance travelled.

Neither Fischer's Model nor the FWQA Model reproduce the effects of longitudinal dispersion based on theoretical knowledge of the fluid mechanics of the process. Therefore, they are descriptive rather than predictive since their dispersion coefficients must be confirmed by

comparison with field data. Theoretical work on longitudinal dispersion has been done by Taylor and Elder, who developed analytical expressions for the dispersion coefficient E under conditions of steady, uniform flow. Holley, Harleman and Fischer (1970) discuss procedures for extending the work of Taylor and Elder to homogeneous estuary flow. With dispersion coefficients based on this work, it is possible to develop a predictive model for the longitudinal dispersion process in estuaries.

Since both Fischer's Model and the FWQA Model are formulated in terms of control volumes, they simulate discrete mass transfers between adjacent volumes directly. They do not attempt to solve the conservation of mass equation, which describes the continuous mass transfer process in a channel; and match boundary conditions at channel intersections in a network. This approach would permit greater flexibility in the selection of numerical solution procedures. The FWQA Model is analogous to an explicit finite difference solution of the conservation of mass equation with appropriate weights on the space derivatives. The two approaches will generate identical equations for the junction concentrations if the FWQA Model is applied to a cascade of channels and junctions of uniform size Δx . One problem with the FWQA Model and explicit finite difference stations is that they are especially prone to numerical dispersion, which is a symptom of poor convergence. Within the context of finite difference solution techniques it is possible to choose high accuracy operators such as the Stone and Brian 6-point implicit scheme. However, there is general difficulty with finite difference schemes at boundaries in a network formulation where concentration itself is not

specified. This was seen in the present study through early work which was aimed at formulating a procedure for matching boundary conditions at channel intersections with the Stone and Brian 6-point explicit scheme. The procedure involved the use of so-called "guard points", or "fictitious points", which resulted in severe computational problems. Numerical error was amplified and the computations became unstable.

For solving the conservation of mass equation in a network formulation, the finite element method appears to be very promising. High accuracy operators can be established, as demonstrated by Price, Cavendish and Varga (1968), and the variable mesh capability of the operators makes them very flexible. Variable mesh spacing is very useful in the vicinity of injection points where the mesh can be refined to resolve steep concentration gradients. Although fine mesh may be desirable for water quality computations, one wants to use a reasonably coarse mesh for the tidal hydraulic computations. This maximizes the hydraulic time step Δt which is proportional to the mesh spacing Δx . To reconcile these differences, separate computational meshes may be set up for the hydraulic and water quality models. At time steps where a water quality solution is desired, geometric parameters and discharges may be interpolated from the hydraulic mesh to the water quality mesh. Interpolation errors should not be too significant, as the variation of water surface elevation and discharge is fairly smooth over the length of a channel.

To simplify both interpolation and network formulation of the hydraulic model, it is desirable to have a hydraulic solution procedure

which generates both water surface elevations and discharges at all mesh points at all time. At channel intersections, compatibility of water surface elevations and continuity of discharges can be written singly in terms of elevations and discharges at the boundary mesh points. The leap-frog finite difference scheme used by Lee and Harleman (1971) is not suited to matching boundary conditions because of the staggered grid shown in Figure 2.2. Either water surface elevation or discharge is available at boundary mesh points, but not both. Therefore, the network hydraulic model is taken from a finite element, implicit formulation by Gunaratnum and Perkins (1970), which was made operational by Wood, Harley and Perkins (1972).

A further advantage of the finite element method is that correct treatment of boundary conditions in the water quality model comes as a direct result of the discretization process, as will be shown in section 3.1.1. There is no need for fictitious points, so that the procedure for matching boundary conditions is straightforward and computationally efficient. Also, formulation of the ocean boundary condition on ebb tide can be clarified and placed on a more rigorous basis.

2.3.3 The Ocean Boundary Condition

For a predictive model of water quality in estuaries, one of the most difficult problems is the ocean boundary condition. Physically, the boundary condition must permit relatively unrestricted movement of mass out of the estuary on ebb tide; however, it must control mass return on flood tide in order to describe the effects of tidal flushing.

To formulate the ocean boundary condition, use is made of the observed fact that the advective mass flux ρQc is usually one or two orders of magnitude larger than the dispersive flux (see Lee and Harleman (1971)). This permits a two-phase boundary condition over a tidal cycle. On ebb tide, specification of dispersive flux provides a weak restraint on advective flux leaving the estuary. The concentration computed at the boundary is affected primarily by transport from upstream. On flood tide, the concentration is specified to provide a relatively strong condition on mass re-entering the estuary.

Both the dispersive flux and concentration formulation must vary dynamically over their portions of the tidal cycle. On ebb tide, dispersive flux must change to accommodate the passage of concentration fronts. On flood tide, the boundary concentration will undergo a transition from a computed ebb slack value to a known ocean value.

Variation of the dispersive flux at the ocean boundary is achieved in the following manner. As each time step of the calculations is completed, an approximation of the dispersive flux at the next time step is formed using its current value and an estimate of its rate of change. The rate of change estimate can be formed by examining the numerical solution itself immediately upstream of the ocean boundary at successive time steps. An analogy may be posed where an observer is placed at the ocean boundary with a valve which controls dispersive flux on ebb tide. He is also equipped with sensors which read out concentrations upstream of the ocean boundary stepwise in time. At a given time step he can compare the current sensor readings with readings at the

previous time step to estimate the rate of change of the concentration gradient adjacent to the boundary. With known cross-sectional areas and dispersion coefficients, he can compute an adjustment to the existing valve setting which will release either more or less dispersive flux over the next time step. In this way, the release of dispersive flux is matched to concentration gradients which are swept towards the ocean boundary on ebb tide. The mechanics of the adjustment procedure in the numerical solution itself are described in section 3.1.2.

Specification of dispersive flux continues through the ebb tide until the time of low water slack. As flood tide begins, concentration is specified at the ocean boundary. The transition of the boundary concentration from its low water slack value to a known ocean value will control the return of mass to the estuary. With the definitions in Figure 2.7, the mass returning to the estuary on flood tide is

$$M_r = \int_{LWS}^{HWS} Q_b c_b dt \quad (2.39)$$

where the mass flux due to dispersion is neglected. The resulting mass can be expressed as a percentage of the mass which left on the previous ebb tide:

$$M_r = r M_{ebb} \quad (2.40)$$

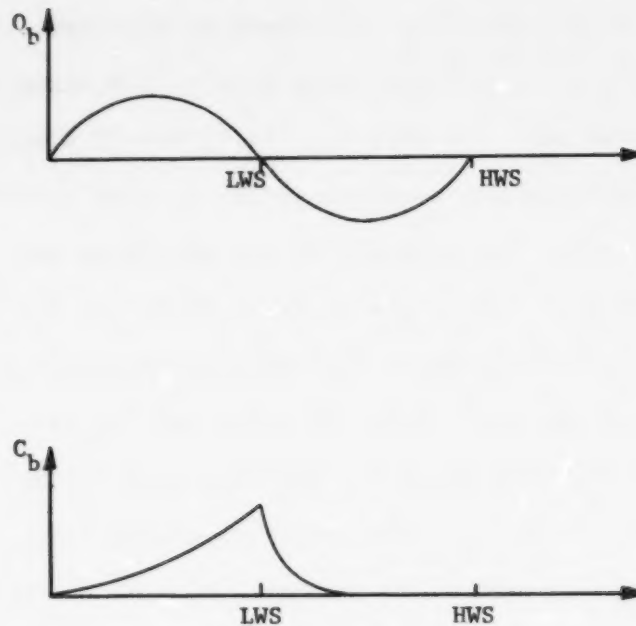


Figure 2.7 Time Variation of Boundary Discharge and Concentration

In certain simplified situations, it is possible to adjust the time rate of change of concentration to achieve a desired per cent return. For example, the discharge may be considered as a sinusoidal function, and the concentration may be assumed to undergo an exponential decay:

$$Q = Q_f + Q_o \sin \sigma t \quad (2.41a)$$

$$c = c_{LWS} e^{-K_o (t - t_{LWS})} \quad (2.41b)$$

Then the mass returning on flood tide is:

$$-r M_{ebb} = \int_{t_{LWS}}^{t_{HWS}} \rho(Q_f + Q_o \sin \sigma t) c_{LWS} e^{-K_o(t-t_{LWS})} dt \quad (2.42)$$

The minus sign on the mass return is required because the flood discharge is defined to be negative. All quantities within the integral are specified except the decay constant K_o . This may be adjusted to yield a desired per cent return r . If one makes the approximations

$$t_{LWS} \approx \frac{T}{2} \quad (2.43a)$$

$$t_{HWS} \approx T \quad (2.43b)$$

the integral may be evaluated to yield:

$$g(K_o) = \frac{\rho Q_f c_{LWS}}{K_o} \left[1 - e^{-\frac{K_o T}{2}} \right] - \frac{\rho Q_o c_{LWS} \sigma}{K_o^2 + \sigma^2} \left[1 + e^{-\frac{K_o T}{2}} \right] + r M_{ebb} = 0 \quad (2.44)$$

An analytic solution of this equation for K_o is difficult, but a numerical solution with a technique such as interval halving is easy to obtain in the computer. Successive estimates of K_o are made until $g(K_o) \approx 0$. One starting point for the solution would be the case of $K_o = 0$, or $c = c_{LWS}$ for the entire flood tide.

$$\lim_{K_o \rightarrow 0} g(K_o) = \frac{\rho Q_f c_{LWS} T}{2} - \frac{\rho Q_o L_o T}{\pi} + r M_{ebb} \quad (2.45)$$

This expression should be strongly negative, implying an excess of mass returning to the estuary. It should be pointed out that the expression might never go negative if a very large slug of waste passed through the ocean boundary on ebb leaving only a residual concentration at low-water slack. Then the approach breaks down, for it is assumed that sufficient concentration remains at the boundary to achieve the desired per cent return.

In dealing with prototype estuaries in practical situations, there is little or no theoretical knowledge available to describe how the ocean boundary concentration should vary under different conditions. For particular estuaries of interest, it is likely that this information will have to be obtained from detailed field studies. Parker, Norris, and Nelson (1972) describe a study in San Francisco Bay where salinities and temperatures were measured at the ocean boundary over two tidal periods of different amplitudes. Their analysis was aimed at the derivation of tidal exchange coefficients rather than a fundamental understanding of how the ocean boundary concentration varies on flood tide. It would seem that the latter objective would be more helpful for subsequent use in mathematical models.

2.3.4 Solution Technique for Multiple Constituents

Current research in estuarine water quality is being directed towards definition of the appropriate constituents for particular problems and the interactions which occur between them. Figure 2.8 illustrates the major feature of the nitrogen cycle as presented by O'Connor and Thomann in Chapter III of TRACOR (1971). The process is

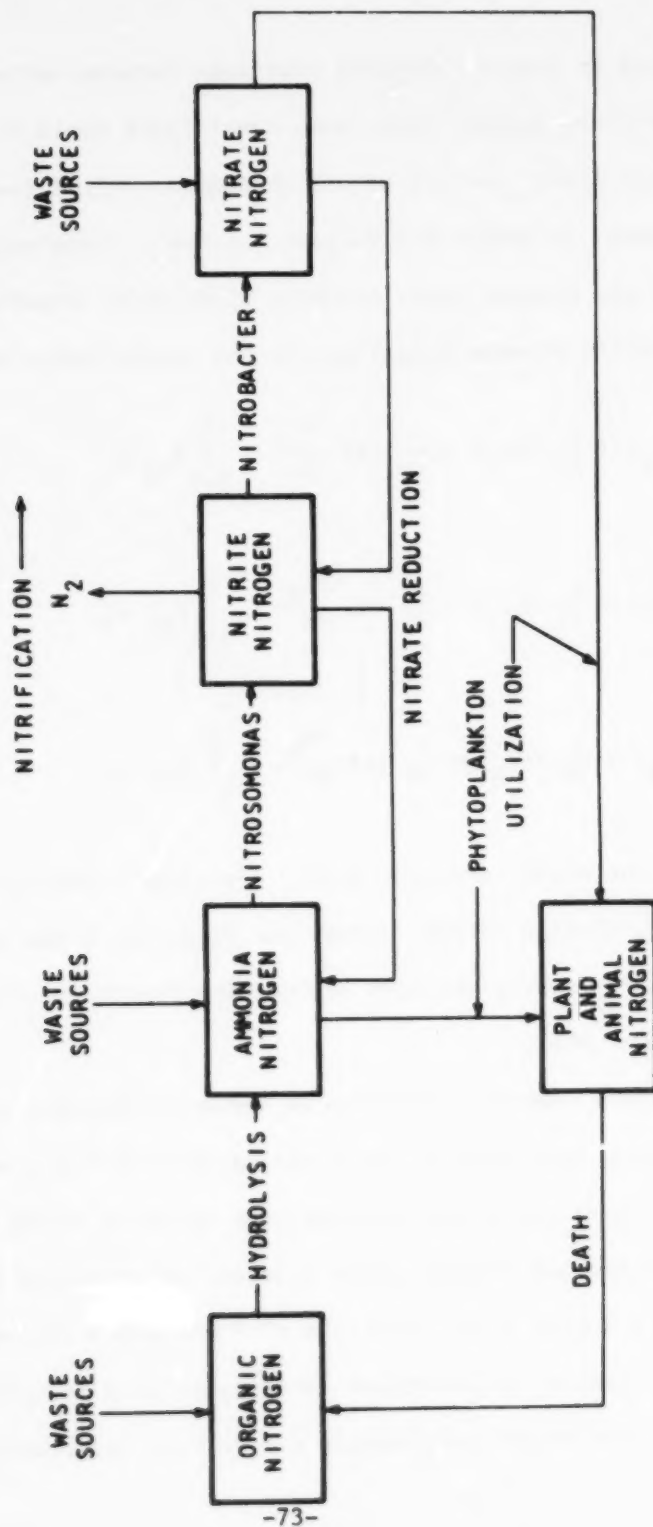


Figure 2.8 Major Features of the Nitrogen Cycle
(from TRACOR (1971), Chapter III by D.J. O'Connor and R.V. Thomann)

that the entire matrix must be included in the solution computations. For one-dimensional problems in particular, it would seem computationally more efficient to arrange the equations so that the solution vector is composed of M sub-vectors, each containing N constituent concentrations at a mesh point. The structure of the coefficient matrix will be a function of the numerical difference operator employed; however, most widely used operators involve three adjacent mesh points. In this case, the set of equations may be written in the matrix form:

$$\begin{bmatrix} \underline{\Lambda}^1 & & & & \underline{\Gamma}^1 \\ & \underline{T}^2 & & & \\ & & \underline{\Lambda}^2 & & \underline{\Gamma}^2 \\ & & & \ddots & \\ & & & & \underline{T}^N & & \underline{\Lambda}^N \end{bmatrix} \begin{bmatrix} \underline{\bar{c}}_1 \\ \underline{\bar{c}}_2 \\ \vdots \\ \underline{\bar{c}}_N \end{bmatrix} = \begin{bmatrix} \underline{B}^1 \\ \underline{B}^2 \\ \vdots \\ \underline{B}^N \end{bmatrix} \quad (2.47)$$

where $\underline{\Lambda}^i$, $\underline{T}^i$, and $\underline{\Gamma}^i$ are $N \times N$ submatrices, $\underline{\bar{c}}_i$ is an $N \times 1$ solution sub-vector of constituent concentrations at mesh point i , and $\underline{B}^i$ is an $N \times 1$ sub-vector on the right-hand side. The coefficient matrix is tri-diagonal in nature, so that the solution procedure need consider only matrix elements within a throw of $2N$ from the main diagonal. The most efficient procedure would be a generalization of the well-known Thomas algorithm to operate directly on the $N \times N$ submatrices $\underline{\Lambda}^i$, $\underline{T}^i$, and $\underline{\Gamma}^i$. However, not too much computation would be involved in using one of the banded equation solvers commonly available in computer program libraries.

Even with the introduction of computational efficiencies, solution of MN simultaneous equations can be a time-consuming task, especially in dynamic computations. Di Toro (1972) has suggested a procedure for sequential reactions where only the distribution of the first constituent need be calculated, and the concentrations of succeeding constituents are calculated by recurrence relationships. The application is limited to reaction processes where the effects of a given constituent are fed forward to succeeding constituents and not backward to previous ones. Therefore, a reaction process which contains feedback loops, such as the one in Figure (2.8), cannot be handled.

It should be pointed out that interaction of constituents is not limited to the reaction processes as described in Equations (2.46). For example, one effect of salinity as a constituent is to increase dispersion in the region of steep gradients and spread out the distribution of other constituents. Also, salinity may increase the saturation concentration of dissolved oxygen. Similarly, temperature affects the reaction coefficient K_1 in the BOD decay process.

In the present study, formulation of solution procedures for the tidal hydraulics and concentration distributions of salinity, temperature, BOD, and DO is based on the notion of feed-forward effects. The equations solved are summarized as follows:

$$\text{Continuity: } \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_L \quad (2.6)$$

$$\text{Momentum: } \frac{\partial}{\partial t}(AU) + \frac{\partial}{\partial x}(QU) = -Ag \left(\frac{\partial z}{\partial x} + \frac{U|U|}{C_z^2 R_h} + \frac{d_c}{\rho} \frac{\partial \rho}{\partial x} \right) \quad (2.48)$$

$$\text{Salinity: } \frac{\partial}{\partial t}(As) + \frac{\partial}{\partial x}(Qs) = \frac{\partial}{\partial x} (AE \frac{\partial s}{\partial x}) \quad (2.2)$$

$$\text{Temperature: } \frac{\partial}{\partial t}(AT) + \frac{\partial}{\partial x}(QT) = \frac{\partial}{\partial x} (AE \frac{\partial T}{\partial x}) - K_T A (T - T_e) \quad (2.3)$$

$$\text{BOD: } \frac{\partial}{\partial t}(AL) + \frac{\partial}{\partial x}(QL) = \frac{\partial}{\partial x} (AE \frac{\partial L}{\partial x}) - K_1 AL \quad (2.4)$$

$$\text{DO: } \frac{\partial}{\partial t}(AC) + \frac{\partial}{\partial x}(QC) = \frac{\partial}{\partial x} (AE \frac{\partial C}{\partial x}) - K_1 AL + K_2 A (C_s - C) \quad (2.5)$$

Computational experience in the present study revealed an interesting problem associated with computing DO concentrations about the saturation concentration C_s . In upstream regions of an estuary where there was no BOD loading, the DO concentrations decreased by about 0.1 - 1.0% per tidal cycle. This decrease is small in comparison with the BOD sink term; however, it led to the appearance of a sizeable oxygen deficit over a large number of tidal cycles.

The problem is caused by round-off error in the computations, which may be shown qualitatively by considering the numerical representation of the storage term in the DO equation:

$$\frac{\partial}{\partial t}(AC) \approx \frac{(AC)^{t+\Delta t} - (AC)^t}{\Delta t}$$

In an estuary, the areas are quite large, reaching 4 to 6 digits. Over a short time step Δt , the storage term involves finding a small difference between large numbers. Inasmuch as standard precision calculations in the IBM 360 and 370 computers are accurate to about 7 digits, it is not surprising that round-off error would accumulate and begin to affect the accuracy of the computed concentrations.

The mass loss through round-off could probably be corrected by doing the computations in double precision; however, this requires increased storage space and execution time. It is easier to reformulate the DO equation in terms of dissolved oxygen deficit (DOD) and continue the computations in standard precision. In regions where BOD loadings are zero, DOD will also be zero and round-off will no longer be a problem. Where BOD loadings are significant, physical error tolerances in the decay and reaeration coefficients K_1 and K_2 will overshadow mass loss by round-off. The DOD equation may be written:

$$\text{DOD: } \frac{\partial}{\partial t}(AD) + \frac{\partial}{\partial x}(QD) = \frac{\partial}{\partial x}(AE \frac{\partial D}{\partial x}) + K_1 AL - K_2 AD \quad (2.49)$$

where

$$D = C_s - C$$

A similar procedure is followed for the temperature equation which is reformulated in terms of temperature excess:

$$\begin{array}{l} \text{Temperature} \\ \text{Excess:} \end{array} \quad \frac{\partial}{\partial x}(AT^e) + \frac{\partial}{\partial x}(QT^e) = \frac{\partial}{\partial x}(AE \frac{\partial T^e}{\partial x}) - K_T AT^e \quad (2.50)$$

where

$$T^e = T - T_e$$

Salinity is a conservative substance; therefore, there are no sink terms to absorb the mass loss due to round-off. Thatcher and Harleman noted small losses of salinity in the course of their studies; however, the losses were not considered significant for practical applications. It is likely that full ocean salinity flowing into the estuary on flood tide tended to overcome losses due to round-off.

The computational procedure for solving the set of equations is as follows. At a given time step, the tidal hydraulics are determined first with the continuity and momentum equations including density effects caused by the longitudinal salinity distribution. The salinity distribution at the previous time step is used, which should not result in significant errors when the time step is reasonably small. This salinity distribution is also used to calculate new, local dispersion coefficients based on the procedure given by Thatcher and Harleman (1972). With these dispersion coefficients the new concentration distributions of salinity, temperature excess, BOD, and DOD are computed sequentially. At present, salinity and temperature do not interact with BOD and DOD; however, effects such as sensitivity of K_1 and K_2 to temperature could be included. Effects of BOD are fed forward to the DOD calculation by entering the computed BOD concentration distribution into the source term of the DOD equation.

The sequential computational procedure allows the use of computer programs which were originally developed for a single constituent. Such programs were developed as part of the present study, where the primary purpose was to consider the network water quality problem for individual constituents without immediate concern for complex coupling in the

reaction processes. With some effort, the programs could be modified to handle an intricately coupled, multiple constituent problem in the manner outlined above.

CHAPTER III

DEVELOPMENT OF THE NUMERICAL SOLUTION TECHNIQUE

3.1 Conservation of Mass Equation

3.1.1 Application of the Method of Weighted Residuals

As indicated in section 2.2.5b, numerical solution based on the concentration distribution equation, Equation (2.21), may not conserve mass. Therefore, development of the numerical solution technique will start with the conservation of mass equation in its primary form.

$$\frac{\partial}{\partial t} (Ac) + \frac{\partial}{\partial x} (Qc) = \frac{\partial}{\partial x} \left(AE \frac{\partial c}{\partial x} \right) + \left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \quad (2.1)$$

The method of weighted residuals is applied by dividing the channel into elements which are connected at nodes or mesh points. The terms in Equation (2.1) are then assumed to vary in a linear manner over the elements as shown in Figure 3.1.

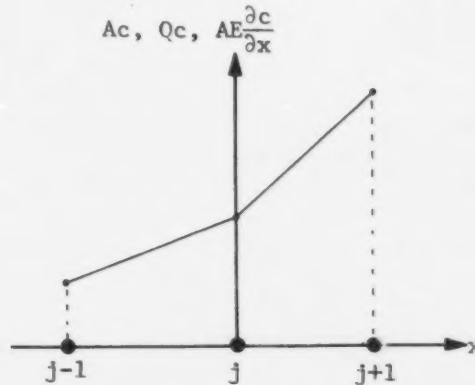


Figure 3.1 Linear Variation of the Equation Terms over the Elements

Higher order polynomial variations could be assumed; however, the linear variation is preferred because it is simple to use and it yields a set of equations which are convenient to interpret physically. Also, the resulting numerical operator strongly resembles the Stone and Brian operator from finite difference techniques. This provides access to a useful body of knowledge in choosing optimum values of element size and time step.

The variations of the equation terms over the length of the channel are expressed in terms of the interpolating functions discussed in section 2.2.5.

$$Ac = \sum_{j=1}^M \phi_j (Ac)_j \quad (3.1a)$$

$$Qc = \sum_{j=1}^M \phi_j (Qc)_j \quad (3.1b)$$

$$AE \frac{\partial c}{\partial x} = \sum_{j=1}^M \phi_j (AE \frac{\partial c}{\partial x})_j \quad (3.1c)$$

$$\left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A = \sum_{j=1}^M \phi_j \left(\left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \right)_j \quad (3.1d)$$

where

ϕ_j = the interpolating function which is associated with node j
in a given element

$(Ac)_j$ = the value of the storage term at mesh point j

and so on

The piecewise linear approximations (3.1) are substituted next into Equation (2.1). A residual R will exist because the approximations do not yield an exact match of the true solution.

$$\begin{aligned} \frac{\partial}{\partial t} \left(\sum_{j=1}^M \phi_j (Ac)_j \right) + \frac{\partial}{\partial x} \left(\sum_{j=1}^M \phi_j (Qc)_j \right) - \frac{\partial}{\partial x} \left(\sum_{j=1}^M \phi_j (AE \frac{\partial c}{\partial x})_j \right) \\ - \sum_{j=1}^M \phi_j \left(\left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \right)_j = R \end{aligned} \quad (3.2)$$

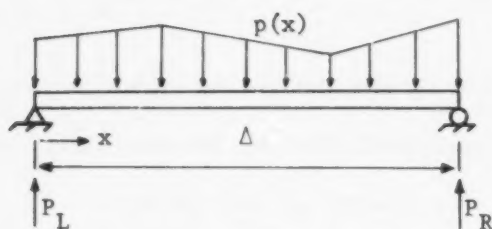
The method of weighted residuals is applied in the form of Galerkin's Method, where the residual is weighted with the interpolating functions, integrated over the length of the channel and set to zero. It is convenient to express the integration as a summation of integrals over the individual elements.

$$\int_L w_i R dx = \sum_E \int \phi_i R dx = 0 \quad i = 1, \dots, m \quad (3.3)$$

In principle there are now M equations for M concentrations at the mesh points. Substituting Equation (3.2) into Equation (3.3) yields:

$$\begin{aligned} \sum_E \int \phi_i \frac{\partial}{\partial t} \left(\sum_{j=1}^M \phi_j (Ac)_j \right) dx + \sum_E \int \phi_i \frac{\partial}{\partial x} \left(\sum_{j=1}^M \phi_j (Qc)_j \right) dx \\ - \sum_E \int \phi_i \frac{\partial}{\partial x} \left(\sum_{j=1}^M \phi_j (AE \frac{\partial c}{\partial x})_j \right) dx - \sum_E \int \phi_i \sum_{j=1}^M \phi_j \left(\left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A \right)_j dx \\ = 0 \quad i = 1, \dots, M \end{aligned} \quad (3.4)$$

Rather than pursue the mathematics of evaluating the integrals immediately, it is helpful to draw an analogy between the individual elements and a simply supported beam subjected to a distributed load. The analogy is shown in Figure 3.2.



$$P_L = \int_0^{\Delta} \frac{\Delta-x}{\Delta} p(x) dx = \int_0^{\Delta} \phi_i p(x) dx$$

$$P_R = \int_0^{\Delta} \frac{x}{\Delta} p(x) dx = \int_0^{\Delta} \phi_{i+1} p(x) dx$$

Figure 3.2. Simply Supported Beam Analogy

In the case of the simple linear elements, the weighting functions ϕ_i in the integrals of Equations (3.4) serve the purpose of prorating the equation terms in concentrated form to the mesh points. This in turn implies that the numerical scheme will conserve mass if it is formulated properly.

The desired result of the integrations in Equations (3.4) is a set of equations for the concentrations at the mesh points. In developing

this set of equations, the following assumptions are introduced.

- (1) The time derivative of the storage term is approximated as a simple difference:

$$\begin{aligned}\frac{\partial}{\partial t}(Ac) &\approx \sum_{j=1}^M \phi_j \frac{\partial}{\partial t} (A_j \bar{c}_j) \\ &\approx \sum_{j=1}^M \phi_j \frac{A_j^{n+1} \bar{c}_j^{n+1} - A_j^n \bar{c}_j^n}{\Delta t}\end{aligned}\quad (3.5)$$

where

$\bar{c}_j^n$ = discrete concentration at mesh point j at time n

This difference approximates the time derivative best at time $t + \frac{\Delta t}{2}$ or $(n + \frac{1}{2}) \Delta t$.

- (2) The remaining terms in the equation are approximated also at time $t + \frac{\Delta t}{2}$ by averaging between times t and $t + \Delta t$. For example, the advective term is:

$$\frac{\partial}{\partial x}(Qc) \approx \frac{1}{2} \frac{\partial}{\partial x} \left(\sum_{j=1}^M \phi_j Q_j^{n+1} \bar{c}_j^{n+1} + \sum_{j=1}^M \phi_j Q_j^n \bar{c}_j^n \right) \quad (3.6)$$

- (3) The source and sink term is divided into a first order decay term and a simple sum of additional sources and sinks:

$$\begin{aligned}\left\{ \frac{r_i}{\rho} + \frac{r_e}{\rho} \right\} A &= -KAc + S \approx -K \frac{1}{2} \left(\sum_{j=1}^M \phi_j A_j^{n+1} \bar{c}_j^{n+1} + \right. \\ &\quad \left. \sum_{j=1}^M \phi_j A_j^n \bar{c}_j^n \right) + S^n + \frac{1}{2}\end{aligned}\quad (3.7)$$

Complex, non-linear interactions of constituents may be handled through the term $S^n + \frac{1}{2}$; however, the present study is restricted to first-order reaction processes. Thus, the decay of BOD is described by setting $K = K_1$, in Equation (3.7). Discharges of BOD are included as additional sources, so that the source and sink term for BOD may be written as

$$\begin{aligned} \left(\frac{r_i}{\rho} + \frac{r_e}{\rho}\right)A_{BOD} &= -K_1AL + q_L L_L + Q_L L_L \delta(x-x_L) \\ &= -K_1AL + S_{BOD} \end{aligned} \quad (3.8)$$

where q_L is a distributed lateral inflow, Q_L is a point lateral inflow, L_L is the BOD concentration of the particular inflow and $\delta(x-x_L)$ is the Dirac delta function. The weighted residual procedure prorates these source terms to the mesh points as shown in Figure 3.2. The point discharge becomes the equivalent of a point load.

Source and sink terms in the DOD equation consist of a BOD sink term, a reaeration term, and discharge terms:

$$\begin{aligned} \left(\frac{r_i}{\rho} + \frac{r_e}{\rho}\right)A_{DOD} &= +K_1AL - K_2AD + (\text{discharges}) \\ &= -K_2AD + S_{DOD} \end{aligned} \quad (3.9)$$

where $S_{DOD} = +K_1AL + (\text{discharges})$

In the DOD equation, the BOD decay term is approximated in the same way as in the BOD equation.

Salinity is a conservative substance, and usually there is

no addition of salinity from discharges. Temperature however is affected by heated discharges and heat loss to the atmosphere.

The source and sink term for temperature excess is

$$\begin{aligned} \left(\frac{r_i}{\rho} + \frac{r_e}{\rho} A \right)_{T,e} &= -K_T A T^e + (\text{discharges}) \\ &= -K_T A T^e + S_T \end{aligned} \quad (3.10)$$

where $S_T = (\text{discharges})$

The heat loss term has the same formulation as the reaeration term, and it is handled in an analogous manner.

(4) In the dispersion term, the coefficient AE is averaged over each element and the concentration is assumed to vary linearly:

$$AE \frac{\partial c}{\partial x} \approx \frac{1}{2} (\overline{AE}^{n+1} \frac{\partial}{\partial x} \sum_{j=1}^m \phi_j \bar{c}_j^{n+1} + \overline{AE}^n \frac{\partial}{\partial x} \sum_{j=1}^m \phi_j \bar{c}_j^n) \quad (3.11)$$

where $\overline{AE}$ = average of AE over an element

$$= \frac{1}{2} \{ (AE)_j^n + (AE)_{j+1}^n \} \text{ for element } j, j+1$$

Assumption (4) is necessary in order to avoid having the dispersive flux integral in Equation (3.4) result in concentration gradients rather than concentrations themselves at the mesh points. A consequence of this assumption about the dispersive flux is a discontinuity at the mesh points. This discontinuity can be shown by integrating the dispersive flux integral by parts:

$$\begin{aligned} \sum_E \int \phi_i \frac{\partial}{\partial x} (AE \frac{\partial c}{\partial x}) dx &= [\phi_i AE \frac{\partial c}{\partial x}]_{x_{i-1}}^{x_i} + [\phi_i AE \frac{\partial c}{\partial x}]_{x_i}^{x_{i+1}} \\ &\quad - \sum_E \int \frac{d\phi_i}{dx} AE \frac{\partial c}{\partial x} dx \quad i = 1, \dots, M \end{aligned} \quad (3.12)$$

Noting that

$$\phi_i = 0 \text{ at } x = x_{i-1} \quad (3.13a)$$

$$\phi_i = 1 \text{ at } x = x_i \quad (3.13b)$$

$$\phi_i = 0 \text{ at } x = x_{i+1} \quad (3.13c)$$

the terms in brackets are

$$AE \frac{\partial c}{\partial x} \bigg|_{\substack{x=x_i \\ \text{element } i-1,i}} - AE \frac{\partial c}{\partial x} \bigg|_{\substack{x=x_i \\ \text{element } i,i+1}} \quad (3.14)$$

$$= (\text{dispersive flux into element } i-1,i) + (\text{dispersive flux into element } i,i+1)$$

In the physical system this sum is zero; however, it is non-zero in the numerical scheme because of the piecewise linear approximation. Nevertheless, the physics of the system are assumed to prevail, and the sum of the two terms is set to zero, except at the boundaries. There, only one of the terms appears, which corresponds to a natural boundary condition in numerical methods which are based on the calculus of variations. This term will be of great use later in section 3.1.2 on the ocean boundary condition.

To simplify the notation, the dispersive fluxes at the boundaries will be written as:

$$\begin{aligned} -AE \frac{\partial c}{\partial x} \bigg|_{x=x_1} &= \text{dispersive at time } (n + \frac{1}{2})\Delta t \text{ flux into upstream boundary} \\ &= \eta_1 \delta_{11} \end{aligned} \quad (3.15a)$$

$$\left. AE \frac{\partial c}{\partial x} \right|_{x=x_M} = \text{dispersive flux at time } (n + \frac{1}{2})\Delta t \text{ into downstream boundary}$$

$$= - \eta_M \delta_{iM} \quad (3.15b)$$

where δ_{i1} and δ_{iM} are Kronecker deltas in matrix notation

Introducing the results of Equations (3.5) through (3.15) into Equations (3.4) yields:

$$\begin{aligned} & \sum_E \int \phi_i \left(\sum_{j=1}^M \phi_j A_j^{n+1-n+1} \bar{c}_j^{n+1} \right) dx + \frac{\Delta t}{2} \sum_E \int \phi_i \left(\sum_{j=1}^M \frac{d\phi_j}{dx} Q_j^{n+1} \bar{c}_j^{n+1} \right) dx \\ & + \frac{\Delta t}{2} \sum_E \bar{A} E^{n+1} \int \frac{d\phi_i}{dx} \left(\sum_{j=1}^M \frac{d\phi_j}{dx} \bar{c}_j^{n+1} \right) dx + \frac{K\Delta t}{2} \sum_E \int \phi_i \left(\sum_{j=1}^M \phi_j A_j^{n+1} \bar{c}_j^{n+1} \right) dx \\ & = \sum_E \int \phi_i \left(\sum_{j=1}^M \phi_j A_j^n \bar{c}_j^n \right) dx - \frac{\Delta t}{2} \sum_E \int \phi_i \left(\sum_{j=1}^M \frac{d\phi_j}{dx} Q_j^n \bar{c}_j^n \right) dx \\ & - \frac{\Delta t}{2} \sum_E \bar{A} E^n \int \frac{d\phi_i}{dx} \left(\sum_{j=1}^M \frac{d\phi_j}{dx} \bar{c}_j^n \right) dx - \frac{K\Delta t}{2} \sum_E \int \phi_i \left(\sum_{j=1}^M \phi_j A_j^n \bar{c}_j^n \right) dx \\ & + \eta_1 \Delta t \delta_{i1} - \eta_M \Delta t \delta_{iM} + \Delta t \sum_E \int \phi_i S^{n+\frac{1}{2}} dx, \quad i = 1, \dots, M \end{aligned} \quad (3.16)$$

Appendix A contains a summary of the values of the integrals in Equations (3.16). With these values, Equations (3.16) may be written in matrix notation as:

$$\underline{A} \underline{\bar{c}}^{n+1} = \underline{D} \underline{\bar{c}}^n + \underline{e} \quad (3.17)$$

Diagram A illustrates a sequence of operations. It shows a grid with labels a^1 , c^1 , b^2 , a^2 , c^2 , b^{M-1} , a^{M-1} , c^{M-1} , b^M , and a^M . Two circles are present, one at the top right and one at the bottom left. Three diagonal lines connect the top row of labels to the bottom row of labels.

$$a^1 = 2f_2 \Delta_{1,2} A_1^{n+1} - f_4^{1,n+1} + f_1^{1,n+1}$$

$$a^i = 2f_2(\Delta_{i-1,i} + \Delta_{i,i+1})A_i^{n+1} + f_1^{i-1,n+1} + f_1^{i,n+1}, \quad 2 \leq i \leq M-1$$

$$a^M = 2f_2 \Delta_{M-1,M} A_M^{n+1} + f_4^{M,n+1} + f_1^{M-1,n+1}$$

$$c^i = f_2 \Delta_{i,i+1} A_{i+1}^{n+1} + f_4^{i+1,n+1} - f_1^{i,n+1}, \quad 1 \leq i \leq M-1$$

$$b^i = f_2 \Delta_{i-1,i} A_{i-1}^{n+1} - f_4^{i-1,n+1} - f_1^{i-1,n+1}, \quad 2 \leq i \leq M$$

and

$$f_1^{i,n+1} = \frac{A_i^{n+1} E_i^{n+1} + A_{i+1}^{n+1} E_{i+1}^{n+1}}{\Delta_{i,i+1}} \frac{\Delta t}{4}$$

$$f_2 = \frac{1}{6} \left(1 + \frac{K\Delta t}{2} \right)$$

$$f_3 = \frac{1}{6} \left(1 - \frac{K\Delta t}{2} \right)$$

$$f_4^{i,n+1} = \frac{Q_i^{n+1} \Delta t}{4}$$

$$\underline{\underline{D}} = \begin{bmatrix} d_a^1 & d_c^1 & & & \\ & d_b^2 & d_a^2 & d_c^2 & \\ & & & & \bigcirc \\ & & & & \\ \bigcirc & & & d_b^{M-1} & d_a^{M-1} & d_c^{M-1} \\ & & & & d_b^M & d_a^M \end{bmatrix}$$

where

$$d_a^1 = 2f_3 \Delta_{1,2} A_1^n + f_4^{1,n} - f_1^{1,n}$$

$$d_a^i = 2f_3 (\Delta_{i-1,i} + \Delta_{i,i+1}) A_i^n - f_1^{i-1,n} - f_1^{i,n}, \quad 2 \leq i \leq M-1$$

$$d_a^M = 2f_3 \Delta_{M-1,M} A_M^n - f_4^{M,n} - f_1^{M-1,n}$$

$$d_c^i = f_3 \Delta_{i,i+1} A_{i+1}^n - f_4^{i+1,n} + f_1^{i,n}, \quad 1 \leq i \leq M-1$$

$$d_b^i = f_3 \Delta_{i-1,i} A_{i-1}^n + f_4^{i-1,n} + f_1^{i-1,n}, \quad 2 \leq i \leq M$$

The vectors $\bar{c}$ and $\underline{e}$ are defined as:

$$\bar{c}^n = \begin{bmatrix} \bar{c}_1 \\ \bar{c}_2 \\ | \\ \bar{c}_{M-1} \\ \bar{c}_M \end{bmatrix} \quad \underline{e} = \begin{bmatrix} \eta_1 \Delta t + (\text{source terms})_1 \\ (\text{source term})_2 \\ | \\ (\text{source terms})_{M-1} \\ -\eta_M \Delta t + (\text{source terms})_M \end{bmatrix}$$

3.1.2 Initial Conditions and Boundary Conditions

To obtain a solution of the conservation of mass equation, it is mathematically necessary to specify an initial condition and two boundary conditions for each reach. In the numerical solution, the initial condition takes the form of beginning concentrations $\bar{c}$ at each of the mesh points. With these specified, the solution can be marched forward in time, subject to the boundary conditions and source terms contained in the vector $\underline{e}$. The most straightforward type of boundary condition to specify is dispersive flux, which is done by evaluating $\eta_1 \Delta t$ and/or $\eta_M \Delta t$.

Specification of concentration at the boundaries is an indirect specification of the advective mass flux ρQc . With the mechanics of computing procedures in mind, the simplest way to specify concentration is to manipulate the matrices of Equation (3.17). For concentration

prescribed at the upstream boundary, row 1 of the coefficient matrix $\underline{A}$ is cleared, the main diagonal element is set to 1.0, and element 1 of the right-hand side is set to the specified concentration. Elements in column 1 of the coefficient matrix are multiplied by the specified concentration and transposed to the right-hand side in their rows. A like procedure may be followed for concentrations prescribed at the downstream boundary.

A third type of boundary condition which may be specified is total flux, or the sum of advective flux and dispersive flux. This is useful where the mass flux through a boundary is known, such as in a river where the waste input at the upstream boundary is a certain number of lbs/day or BTU/day. At the head of tide in an estuary, the mass flowing through the boundary is zero. In order to specify total flux, it is necessary to return to Equation (3.4) and integrate the advective flux integral by parts:

$$\begin{aligned} \sum_E \int \phi_i \frac{\partial}{\partial x} (Qc) dx &= [\phi_i Qc]_{x_{i-1}}^{x_i} + [\phi_i Qc]_{x_i}^{x_{i+1}} \\ &\quad - \sum_E \int \frac{\partial \phi_i}{\partial x} Qc dx, \quad i = 1, \dots, M \end{aligned} \quad (3.18)$$

By arguments similar to those for the dispersive flux integral, the terms in brackets in Equation (3.18) cancel at interior mesh points, but are non-zero at the boundaries. The result is:

$$\sum_E \int \phi_i \frac{\partial}{\partial x} (Qc) dx = - Qc|_{x=0} + Qc|_{x=x_M} - \sum_E \int \frac{\partial \phi_i}{\partial x} Qc dx \quad (3.19)$$

Thus, the integration by parts has no effect at interior mesh points, and modifications of the matrix elements of Equation (3.17) are confined to the boundaries. Denoting the modified elements by a prime:

$$a_1^{1'} = 2f_2 \Delta_{1,2} A_1^{n+1} + f_4^{1,n+1} + f_1^{1,n+1}$$

$$a_M^{M'} = 2f_2 \Delta_{M-1,M} A_M^{n+1} - f_4^{M,n+1} + f_1^{M-1,n+1}$$

$$d_a^{1'} = 2f_3 \Delta_{1,2} A_1^n - f_4^{1,n} - f_1^{1,n}$$

$$d_a^{M'} = 2f_3 \Delta_{M-1,M} A_M^n + f_4^{M,n} - f_1^{M-1,n}$$

$$e_1' = (\text{total flux})_1 \Delta t + (\text{source terms})_1$$

$$e_m' = (\text{total flux})_M \Delta t + (\text{source terms})_M$$

The physical interpretation of this result is that the following equalities have been added to Equations (3.17).

$$\frac{\Delta t}{2} (Q_1^{n+1} \bar{c}_1^{n+1} + Q_1^n \bar{c}_1^n) = (\text{advective flux})_1 \Delta t \quad (3.20a)$$

$$\frac{\Delta t}{2} (Q_M^{n+1} \bar{c}_M^{n+1} + Q_M^n \bar{c}_M^n) = (\text{advective flux})_M \Delta t \quad (3.20b)$$

The boundary condition is imposed by evaluating a total flux term instead of a dispersive flux term in the boundary equations.

The ocean boundary condition is handled by checking the discharge at a given time step. If discharge is into the boundary, concentration

of the inflowing water is specified. If discharge is out of the boundary, dispersive flux is specified. After the computations at a given time step are completed, an approximation is formed for the dispersive flux at the next time step. At the upstream boundary, this approximation is given by Equation (3.21):

$$\eta_1(t + \frac{3\Delta t}{2}) = \eta_1(t + \frac{\Delta t}{2}) + \left. \frac{\partial \eta_1}{\partial t} \right|_{t + \frac{\Delta t}{2}} \Delta t \quad (3.21)$$

The quantity $\eta_1(t + \frac{\Delta t}{2})$ is known and the rate of change $\left. \frac{\partial \eta_1}{\partial t} \right|_{t + \frac{\Delta t}{2}}$ may be estimated from solution information retained in the computer:

$$\begin{aligned} \left. \frac{\partial \eta_1}{\partial t} \right|_{t + \frac{\Delta t}{2}} \Delta t &= \frac{\partial}{\partial t} (-AE \frac{\partial c}{\partial x}) \Big|_{t + \frac{\Delta t}{2}} \Delta t \\ &\approx - \left[\frac{(AE)_1^{n+1} + (AE)_2^{n+1}}{2\Delta_{1,2}} (\bar{c}_2^{n+1} - \bar{c}_1^{n+1}) - \frac{(AE)_1^n + (AE)_2^n}{2\Delta_{1,2}} (\bar{c}_2^n - \bar{c}_1^n) \right] \end{aligned} \quad (3.22)$$

Noting that f_1^1 is available at times t and $t + \Delta t$:

$$\eta_1(t + \frac{3\Delta t}{2}) = \eta_1(t + \frac{\Delta t}{2}) - \frac{2}{\Delta t} \{ f_1^{1,n+1} (\bar{c}_2^{n+1} - \bar{c}_1^{n+1}) - f_1^{1,n} (\bar{c}_2^n - \bar{c}_1^n) \} \quad (3.23)$$

By a similar development, the dispersive flux into the downstream boundary may be approximated as:

$$\begin{aligned} -\eta_M(t + \frac{3\Delta t}{2}) &= -\eta_M(t + \frac{\Delta t}{2}) + \frac{2}{\Delta t} [f_1^{M-1,n+1} (\bar{c}_M^{n+1} - \bar{c}_{M-1}^{n+1}) \\ &\quad - f_1^{M-1,n} (\bar{c}_M^n - \bar{c}_{M-1}^n)] \end{aligned} \quad (3.24)$$

3.1.3 Mass Conservation Properties

It was noted in section (3.1.1) that the weighted residual equations for the simple linear element distribute the terms of the conservation of mass equation to the mesh points in the same way that loads on a simply supported beam are distributed to the supports. The purpose of this section is to show that when the contributions to all the mesh points are summed, the numerical scheme conserves mass. A simple way to perform this summation is to add together all of the equations represented by the matrix equation (3.17). The easiest technique is to sum the columns of $\underline{A}$ and $\underline{D}$, which are multiplied by the concentrations in the corresponding rows of $\underline{c}^{n+1}$ and $\underline{c}^n$, and then sum the matrix elements $\underline{e}$. The results are as follows:

Column 1 of $\underline{A} \underline{c}^{n+1}$:

$$\begin{aligned}
 (a^1 + b^2) \underline{c}_1^{n+1} &= (2f_2 \Delta_{1,2} A_1^{n+1} - f_4^{1,n+1} + \cancel{f_1^{1,n+1}} \\
 &\quad + f_2 \Delta_{1,2} A_1^{n+1} - f_4^{1,n+1} - \cancel{f_1^{1,n+1}}) \underline{c}_1^{n+1} \\
 &= (1 + \frac{K\Delta t}{2}) \frac{\Delta_{1,2}}{2} A_1^{n+1} \underline{c}_1^{n+1} - \frac{Q_1^{n+1} \underline{c}_1^{n+1} \Delta t}{2} \quad (3.25)
 \end{aligned}$$

Column i of $\underline{A} \underline{c}^{-n+1}$: ($i \leq 2 \leq M-1$)

$$\begin{aligned}
 (c^{i-1} + a^i + b^{i+1}) \underline{c}_i^{-n+1} &= (f_2 \Delta_{i-1,i} A_i^{n+1} + \cancel{f_4^{i,n+1}} - \cancel{f_1^{i,n+1}} \\
 &\quad + 2f_2 (\Delta_{i-1,i} + \Delta_{i,i+1}) A_i^{n+1} + \cancel{f_1^{i,n+1}} + \cancel{f_1^{i,n+1}} \\
 &\quad + f_2 \Delta_{i,i+1} A_i^{n+1} - \cancel{f_4^{i,n+1}} - \cancel{f_1^{i,n+1}}) \underline{c}_i^{-n+1} \\
 &= (1 + \frac{K\Delta t}{2}) \frac{\Delta_{i-1,i} + \Delta_{i,i+1}}{2} A_i^{n+1} \underline{c}_i^{-n+1} \quad (3.26)
 \end{aligned}$$

Column M of $\underline{A} \underline{c}^{-n+1}$:

$$\begin{aligned}
 (c^{M-1} + a^M) \underline{c}_M^{-n+1} &= (f_2 \Delta_{M-1,M} A_M^{n+1} + f_4^{M,n+1} - \cancel{f_1^{M,n+1}} \\
 &\quad + 2f_2 \Delta_{M-1,M} A_M^{n+1} + f_4^{M,n+1} + \cancel{f_1^{M,n+1}}) \underline{c}_M^{-n+1} \\
 &= (1 + \frac{K\Delta t}{2}) \frac{\Delta_{M-1,M}}{2} A_M^{n+1} \underline{c}_M^{-n+1} + \frac{0_M^{n+1} \underline{c}_M^{-n+1} \Delta t}{2} \quad (3.27)
 \end{aligned}$$

Column 1 of $\underline{D} \underline{c}^{-n}$:

$$\begin{aligned}
 (d_a^1 + d_b^2) \underline{c}_1^{-n} &= (2f_3 \Delta_{1,2} A_1^n + f_4^{1,n} - \cancel{f_1^{1,n}} \\
 &\quad + f_3 \Delta_{1,2} A_1^n + f_4^{1,n} + \cancel{f_1^{1,n}}) \underline{c}_1^{-n} \\
 &= (1 - \frac{K\Delta t}{2}) \frac{\Delta_{1,2}}{2} A_1^n \underline{c}_1^{-n} + \frac{0_1^n \underline{c}_1^{-n} \Delta t}{2} \quad (3.28)
 \end{aligned}$$

Column i of $\underline{D} \underline{c}^n$: ($i \leq 2 \leq M-1$)

$$\begin{aligned}
 (d_c^{i-1} + d_a^i + d_b^{i+1}) \bar{c}_i^n &= (f_3 \Delta_{i-1,i} A_i^n - \cancel{f_4^{i,n}} + \cancel{f_1^{i-1,n}} \\
 &\quad + 2f_3(\Delta_{i-1,i} + \Delta_{i,i+1}) A_i^n - \cancel{f_1^{i-1,n}} - \cancel{f_1^{i,n}} \\
 &\quad + f_3 \Delta_{i,i+1} A_i^n + \cancel{f_4^{i,n}} + \cancel{f_1^{i,n}}) \bar{c}_i^n \\
 &= (1 - \frac{K\Delta t}{2}) \frac{\Delta_{i-1,i} + \Delta_{i,i+1}}{2} A_i^n \bar{c}_i^n \quad (3.29)
 \end{aligned}$$

Column M of $\underline{D} \underline{c}^n$:

$$\begin{aligned}
 (d_c^{M-1} + d_a^M) \bar{c}_M^n &= (f_3 \Delta_{M-1,M} A_M^{n+1} - \cancel{f_4^{M,n}} + \cancel{f_1^{M-1,n}} \\
 &\quad + 2f_3 \Delta_{M-1,M} A_M^{n+1} - \cancel{f_4^{M,n}} - \cancel{f_1^{M-1,n}}) \bar{c}_M^n \\
 &= (1 - \frac{K\Delta t}{2}) \frac{\Delta_{M-1,M}}{2} A_M^n \bar{c}_M^n - \frac{Q_M^n \bar{c}_M^n \Delta t}{2} \quad (3.30)
 \end{aligned}$$

Sum of e_i :

$$\sum_{i=1}^M e_i = \eta_1 \Delta t - \eta_M \Delta t + \sum_{j=1}^M (\text{source terms})_j \quad (3.31)$$

Summing over all the mesh points and accumulating the storage and decay terms by channel elements $\Delta_{i,i+1}$ yields:

$$\begin{aligned}
& \sum_{i=1}^{M-1} \Delta_{i,i+1} \left(\frac{A_i^{n+1} c_i^{n+1} + A_{i+1}^{n+1} c_{i+1}^{n+1}}{2} \right) = \sum_{i=1}^{M-1} \Delta_{i,i+1} \left(\frac{A_i^n c_i^n + A_{i+1}^n c_{i+1}^n}{2} \right) \\
& - K \Delta t \sum_{i=1}^{M-1} \Delta_{i,i+1} \left(\frac{A_i^{n+1} c_i^{n+1} + A_i^n c_i^n + A_{i+1}^{n+1} c_{i+1}^{n+1} + A_{i+1}^n c_{i+1}^n}{4} \right) \\
& + \Delta t \left(\frac{Q_1^{n+1} c_1^{n+1} + Q_1^n c_1^n}{2} \right) + \eta_1 \Delta t - \Delta t \left(\frac{Q_M^{n+1} c_M^{n+1} + Q_M^n c_M^n}{2} \right) - \eta_M \Delta t \\
& + \sum_{i=1}^M (\text{source terms})_i \tag{3.32}
\end{aligned}$$

The terms in Equation (3.32) define the mass balance:

$$\begin{aligned}
& \left[\begin{array}{c} \text{mass in the} \\ \text{channel at} \\ \text{time } t + \Delta t \end{array} \right] = \left[\begin{array}{c} \text{mass in the} \\ \text{channel at} \\ \text{time } t \end{array} \right] - \left[\begin{array}{c} \text{decay of mass} \\ \text{over the} \\ \text{time step } \Delta t \end{array} \right] \\
& + \left[\begin{array}{c} \text{total inward} \\ \text{flux at the} \\ \text{upstream boundary} \end{array} \right] + \left[\begin{array}{c} \text{total inward} \\ \text{flux at the} \\ \text{downstream boundary} \end{array} \right] + \left[\begin{array}{c} \text{source} \\ \text{terms} \end{array} \right] \tag{3.33}
\end{aligned}$$

This mass balance was achieved with the assumption that dispersive flux is specified at both boundaries. For total flux specified at one or both boundaries, the identities of Equations (3.20) may be added to Equation (3.32) and the mass balance is maintained. If concentration is specified at either the upstream or downstream boundary, the weighted residual equation for the boundary mesh point is no longer needed, and it is replaced by a simple statement of the specified concentration. Therefore, the summation procedure outlined above will involve one or two less equations. Mass balance will be achieved once again, but

rather than repeat the exercise, the result for concentration specified at the upstream boundary will be stated directly as an example.

$$\begin{aligned}
& \left(\frac{A_1^{n+1} \bar{c}_1^{n+1}}{6} + \frac{A_2^{n+1} \bar{c}_2^{n+1}}{3} \right) \Delta_{1,2} + \sum_{i=2}^{M-1} \Delta_{i,i+1} \frac{A_i^{n+1} \bar{c}_i^{n+1} + A_{i+1}^{n+1} \bar{c}_{i+1}^{n+1}}{2} = \\
& \left(\frac{A_1^n \bar{c}_1^n}{6} + \frac{A_2^n \bar{c}_2^n}{3} \right) \Delta_{1,2} + \sum_{i=2}^{M-1} \Delta_{i,i+1} \frac{A_i^n \bar{c}_i^n + A_{i+1}^n \bar{c}_{i+1}^n}{2} \\
& - K \Delta t \left(\frac{1}{6} \frac{A_1^{n+1} \bar{c}_1^{n+1} + A_1^n \bar{c}_1^n}{2} + \frac{1}{3} \frac{A_2^{n+1} \bar{c}_2^{n+1} + A_2^n \bar{c}_2^n}{2} \right. \\
& \left. + \sum_{i=2}^{M-1} \Delta_{i,i+1} \frac{A_i^{n+1} \bar{c}_i^{n+1} + A_i^n \bar{c}_i^n + A_{i+1}^{n+1} \bar{c}_{i+1}^{n+1} + A_{i+1}^n \bar{c}_{i+1}^n}{4} \right) \\
& + \frac{\Delta t}{2} \left(\frac{Q_1^{n+1} \bar{c}_1^{n+1} + Q_2^{n+1} \bar{c}_2^{n+1}}{2} + \frac{Q_1^n \bar{c}_1^n + Q_2^n \bar{c}_2^n}{2} \right) \\
& - \frac{\Delta t}{2} \left(\frac{A_1^{n+1} E_1^{n+1} + A_2^{n+1} E_2^{n+1}}{2} \cdot \frac{\bar{c}_2^{n+1} - \bar{c}_1^{n+1}}{\Delta_{1,2}} + \frac{A_1^n E_1^n + A_2^n E_2^n}{2} \cdot \frac{\bar{c}_2^n - \bar{c}_1^n}{\Delta_{1,2}} \right) \\
& - \Delta t \frac{Q_M^{n+1} \bar{c}_M^{n+1} + Q_M^n \bar{c}_M^n}{2} - r_M \Delta t + \sum_{i=2}^M (\text{source terms})_i
\end{aligned} \tag{3.34}$$

Then, the mass balance is:

$$\begin{aligned}
 & \left[\begin{array}{l} \text{mass at mesh} \\ \text{point 2 and} \\ \text{downstream} \\ \text{at time } t + \Delta t \end{array} \right] = \left[\begin{array}{l} \text{mass at mesh} \\ \text{point 2 and} \\ \text{downstream} \\ \text{at time } t \end{array} \right] - \left[\begin{array}{l} \text{decay of mass} \\ \text{at mesh point 2} \\ \text{and downstream} \\ \text{over time step } \Delta t \end{array} \right] \\
 & + \left[\begin{array}{l} \text{total inward} \\ \text{flux assigned} \\ \text{to mesh point 2} \end{array} \right] + \left[\begin{array}{l} \text{total inward} \\ \text{flux at the} \\ \text{downstream boundary} \end{array} \right] + \left[\begin{array}{l} \text{source terms at} \\ \text{mesh point 2 and} \\ \text{downstream} \end{array} \right]
 \end{aligned}$$

A similar result will be obtained for concentration specified at the downstream boundary.

3.1.4 Convergence Criteria

Even though the numerical scheme developed in the preceding sections conserves mass, there is no assurance that it will be able to produce the correct concentration distribution. This ability is known as the convergence of the scheme. The much-discussed problem of numerical dispersion is a symptom of poor convergence, which results from the choice of network scale Δx and time step Δt . The convergence properties of the numerical scheme as it stands, with variable area, discharge, and dispersion coefficients are extremely difficult, if not impossible, to determine. Therefore, it is necessary to introduce some simplifications. Taking constant, representative values of the equation coefficients A , Q , and E , and specifying a uniform element size Δx , the weighted residuals scheme developed above becomes identical to the 6-point finite difference scheme proposed by Stone and Brian (1963) for solving the convective diffusion equation without decay. (See Figure 2.1).

Similarity of the two schemes is very fortunate in that the convergence analysis presented by Stone and Brian can be expanded easily to include first order decay, and it can be applied directly to the weighted residuals scheme.

The basic principle of the convergence analysis is that a Fourier series representation of the exact, continuous concentration distribution must be closely matched by a second series which approximates the numerical solution. The convective diffusion equation including first order decay is

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} = E \frac{\partial^2 c}{\partial x^2} - Kc \quad (3.36)$$

By direct substitution one can show that Equation (3.36) is satisfied by the following Fourier series:

$$c(x,t) = \sum_{\omega=1}^{\infty} A_{\omega} e^{-(\omega^2 E + K)t} e^{i\omega(x-Ut)} \quad (3.37)$$

where

$$\omega = \frac{2\pi}{L} = \text{wave number}$$

$$L = \text{wave length}$$

Equation (3.37) will be a solution of Equation (3.36) if the boundary conditions are appropriate and the initial condition is composed of harmonics with wave number ω . Physically, Equation (3.37) consists of a series of waves propagating at velocity U and being damped by dispersion and decay. High wave number harmonics experience greater damping by dispersion than low wave number harmonics.

Proceeding to the numerical solution, the discrete concentrations at mesh points in the x-t plane may be described by a second series:

$$\bar{c}_j^n = \sum_{\omega=1}^{M-2} A_{\omega} \xi^n e^{i\omega j \Delta x} \quad (3.38)$$

where M = total number of mesh points

and ξ = a complex constant determined by entering the series into the equation for discrete concentrations which is represented by a computational molecule such as the one in Figure (2.1)

$$= \frac{s + ki}{q + ri}$$

The complex constant ξ may be converted to polar form:

$$\xi = \rho e^{-i\omega U \phi \Delta t} \quad (3.39)$$

where

$$\rho^2 = \frac{s^2 + k^2}{q^2 + r^2}$$

and

$$\phi = \frac{1}{-\omega U \Delta t} (\tan^{-1} \frac{k}{s} - \tan^{-1} \frac{r}{q})$$

Substituting Equation (3.39) into Equation (3.38) yields:

$$\bar{c}_j^n = \sum_{\omega=1}^{M-2} A_{\omega} \rho^n e^{i\omega(j \Delta x - U \phi n \Delta t)} \quad (3.40)$$

The similarity of Equations (3.37) and (3.40) is apparent. Convergence of the numerical solution to the true solution will be achieved as the ratios of the damping and wave celerity in the numerical solution series and the Fourier solution series approach unity:

$$\begin{aligned}
R_1 &= \frac{\text{numerical wave damping}}{\text{Fourier wave damping}} \\
&= \frac{\rho^n}{e^{-(\omega^2 E + K)t}} \\
&\approx 1 \text{ for convergence}
\end{aligned} \tag{3.41}$$

and

$$\begin{aligned}
R_2 &= \frac{\text{numerical wave celerity}}{\text{Fourier wave celerity}} \\
&= \phi \\
&\approx 1 \text{ for convergence}
\end{aligned} \tag{3.42}$$

The definitions of the ratios R_1 and R_2 are valid for any numerical scheme. For a particular scheme, the complex constant ξ defines the polar parameters ρ and ϕ , and hence R_1 and R_2 . When the method of weighted residuals is applied to Equation (3.36) and the series of Equation (3.38) is substituted for the discrete mesh point concentrations, the complex constant ξ is defined as follows.

$$\xi = \frac{s + ki}{q + ri} \tag{3.34}$$

where

$$s = \left(\frac{2}{3} - \frac{\gamma}{6}\right) + \left(\frac{1}{3} - \frac{\gamma}{6}\right) \cos \omega \Delta x - 2\alpha \sin^2 \frac{\omega \Delta x}{2}$$

$$k = -\frac{\beta}{2} \sin \omega \Delta x$$

$$q = \left(\frac{2}{3} + \frac{\gamma}{6}\right) + \left(\frac{1}{3} + \frac{\gamma}{6}\right) \cos \omega \Delta x + 2\alpha \sin^2 \frac{\omega \Delta x}{2}$$

$$r = \frac{\beta}{2} \sin \omega \Delta x$$

and

$$\alpha = \frac{E\Delta t}{\Delta x^2}$$

$$\beta = \frac{U\Delta t}{\Delta x}$$

$$\gamma = K\Delta t$$

For the purposes of developing convergence criteria, the most demanding test of a numerical scheme is the propagation of a slug load or a steep front where $E \approx 0$ and $K \approx 0$. Damping of the higher harmonics in particular will be nominal, and excessive values of the velocity factor ϕ will cause rapid deterioration of the solution. The weighted residuals scheme has the highly desirable property that $R_1 \rightarrow 1$ as $E \rightarrow 0$ and $K \rightarrow 0$. It remains to investigate the behavior of the velocity factor ϕ . Figure 3.3 is a plot of ϕ versus $\omega\Delta x$ for $\alpha = \beta = 0$. The highest numerical accuracy and best convergence will be obtained if $0.9 \leq \phi \leq 1.0$. This condition can be guaranteed if the following criteria are met:

$$\frac{U\Delta t}{\Delta x} \leq 1 \quad (3.44)$$

and

$$\omega\Delta x \leq 1 \quad (3.45)$$

Figure 3.4 shows the effect on ϕ of increasing α while β is held constant at its upper limit of 1.0. To maintain $\phi \approx 1.0$, an additional criterion is suggested.

$$\frac{E\Delta t}{\Delta x^2} \leq 0.5 \quad (3.46)$$

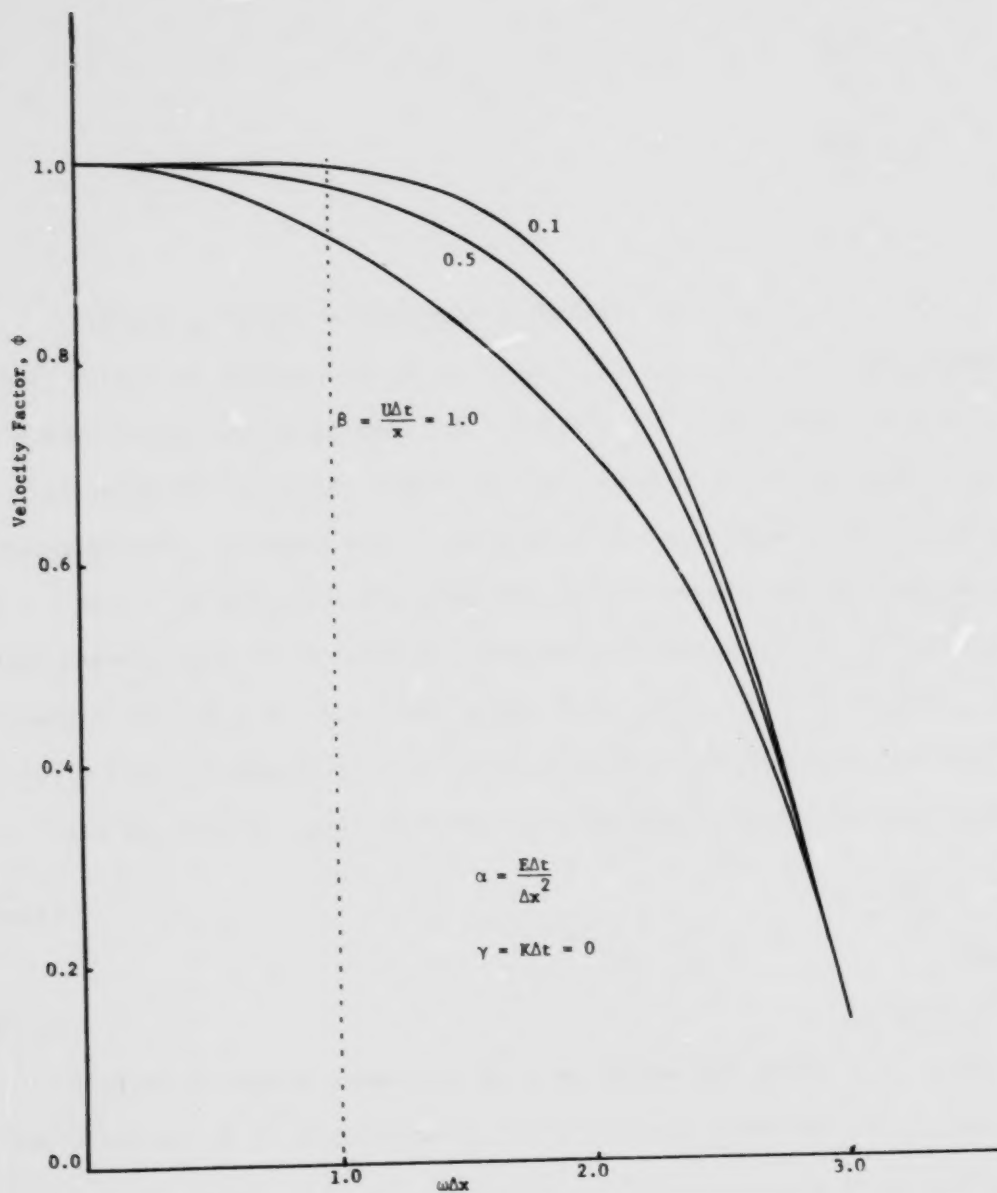


Figure 3.3 Velocity Factor ϕ for $\alpha = \gamma = 0$

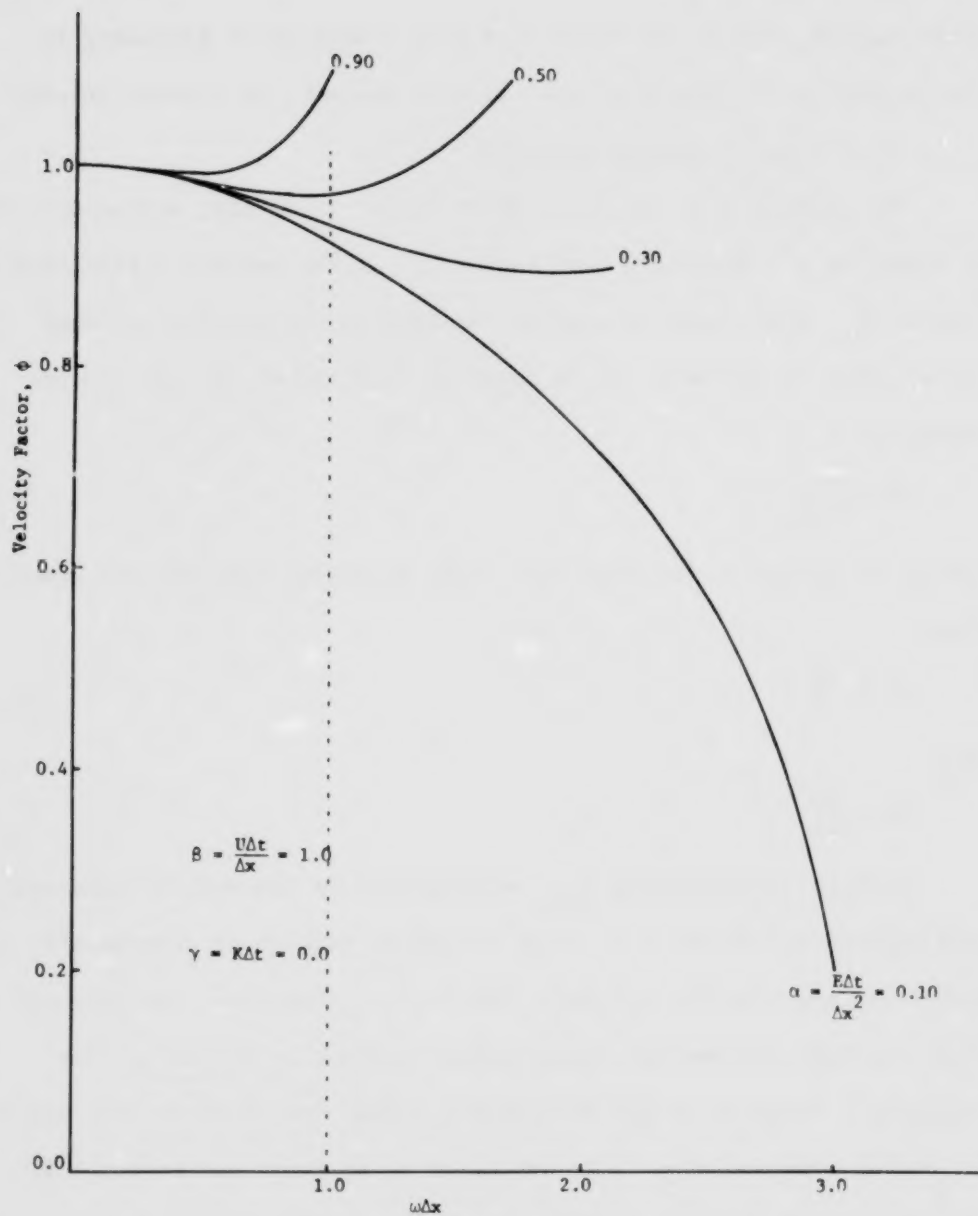


Figure 3.4 Velocity Factor ϕ for $R = 1.0$ and $\gamma = 0.0$

Practical experience has shown that this criterion is secondary in importance to the previous two. If they are met, it usually is also.

3.1.5 Discretization Criteria

The missing piece of information needed to develop a procedure for choosing Δx and Δt is the wave number ω . If the maximum significant wave number $\omega_{\max}$ were known at a given location in the channel, a local upper limit on the value of Δx could be established through the inequality

$$\Delta x \leq \frac{1}{\omega_{\max}} \quad (3.45)$$

Then, the length of the time step could be set by applying the inequalities

$$\Delta t \leq \frac{\Delta x}{U} \quad (3.44)$$

and

$$\Delta t \leq \frac{\Delta x^2}{2E} \quad (3.46)$$

A means of estimating $\omega_{\max}$ is suggested by the work of Gunaratnam and Perkins (1970) who considered a similar problem in discretizing a numerical solution for unsteady flow in open channels. The approach is based on some fundamental input-output concepts in linear systems analysis. Equation (3.36) describes a linear system which will yield an output response when it is subjected to an input excitation. The input excitation may be an injection of mass and the output response is the ensuing concentration distribution. If the spectral density of the input is known, the spectral density of the output can be determined, and a wave number $\omega_{\max}$ can be defined beyond which the area

under the spectral density curve may be neglected.

In general, the input spectral density is not known; it will depend on the nature of the mass injection. As a very conservative assumption, the excitation will be taken as an instantaneous injection of a unit quantity of mass. This is the unit impulse for which the spectral density is of unit strength over all wave numbers from 0 to $\pm \infty$. Continuous injections can be viewed as an integration of instantaneous injections, and the high wave number content of the concentration response will be equal to or less than that of the impulse response.

A second reason for choosing the unit impulse as the excitation function is that the spectral density of the concentration response may be calculated by the simple relation

$$S(\omega, x) = |H(\omega, x)|^2 \quad (3.47)$$

where

$S(\omega, x)$ = spectral density as a function of wave number ω and distance x

$H(\omega, x)$ = complex frequency response as a function of ω and x
where ω is related to frequency through the relation
 $\sigma = \omega U$

The impulse response of Equation (3.36) is a well-known solution for the concentration distribution resulting from an instantaneous injection of unit mass. The complex frequency response $H(\omega, x)$ can be obtained by transforming the impulse response from the time domain to the frequency domain by means of a Fourier integral. Alternatively, it can be derived directly, as in Appendix B, which gives a detailed derivation of the

spectral density.

$$^0S(\omega, x) = \frac{S(\omega, x)}{S(0, x)} \quad (3.48)$$

From Appendix B, the expression for the normalized spectral density downstream of an injection point is

$$^0S(\omega, x) = \left(\frac{r_o}{r}\right) e^{\{r_o - r \cos \theta\} \frac{Ux}{E}}, x > 0 \quad (3.49)$$

where

$$r = \left[\left(1 + \frac{4KE}{U^2}\right)^2 + \left(\frac{4\omega E}{U}\right)^2 \right]^{1/4}$$

$$r_o = \left[1 + \frac{4KE}{U^2} \right]^{1/2}$$

$$\theta = \frac{1}{2} \tan^{-1} \left(\frac{\frac{4\omega E}{U}}{1 + \frac{4KE}{U^2}} \right)$$

Figure 3.5 is a plot of the normalized spectral density at various distances from the injection point. As distance increases, the spectral density moves to the left, indicating decreased contribution of high wave numbers. Physically, this is to be expected. As a concentration slug moves downstream, dispersion will broaden and flatten it, causing higher harmonics to be damped out.

At a given dimensionless distance $\frac{Ux}{E}$ from the injection point, the maximum significant wave number $\omega_{\max}$ is taken from the value of $\frac{4\omega E}{U}$ where the normalized spectral density $^0S(\omega, x)$ drops below some arbitrarily assigned cutoff level. For present purposes, a 5% cutoff

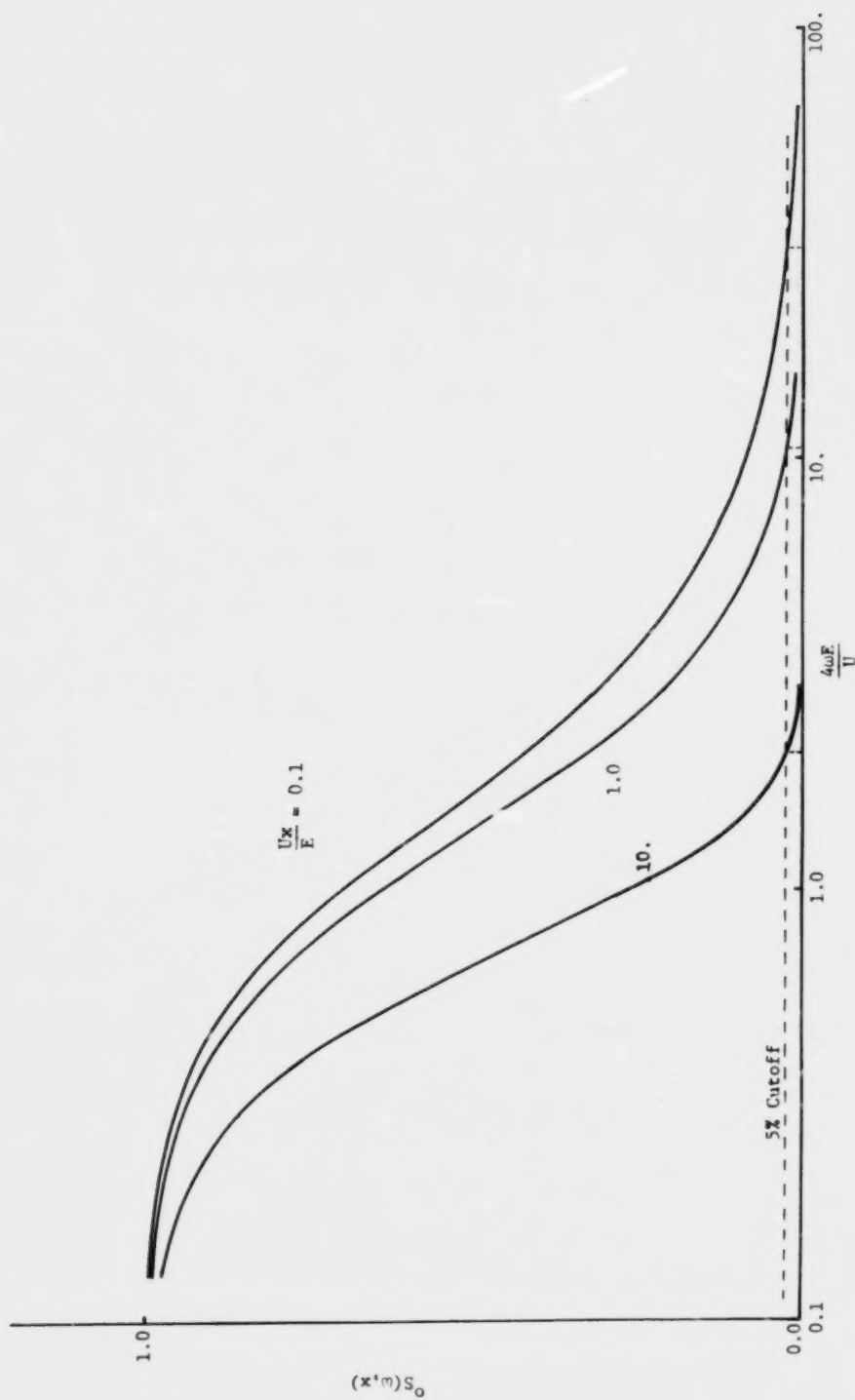


Figure 3.5 Normalized Spectral Density $S(\omega, x)$

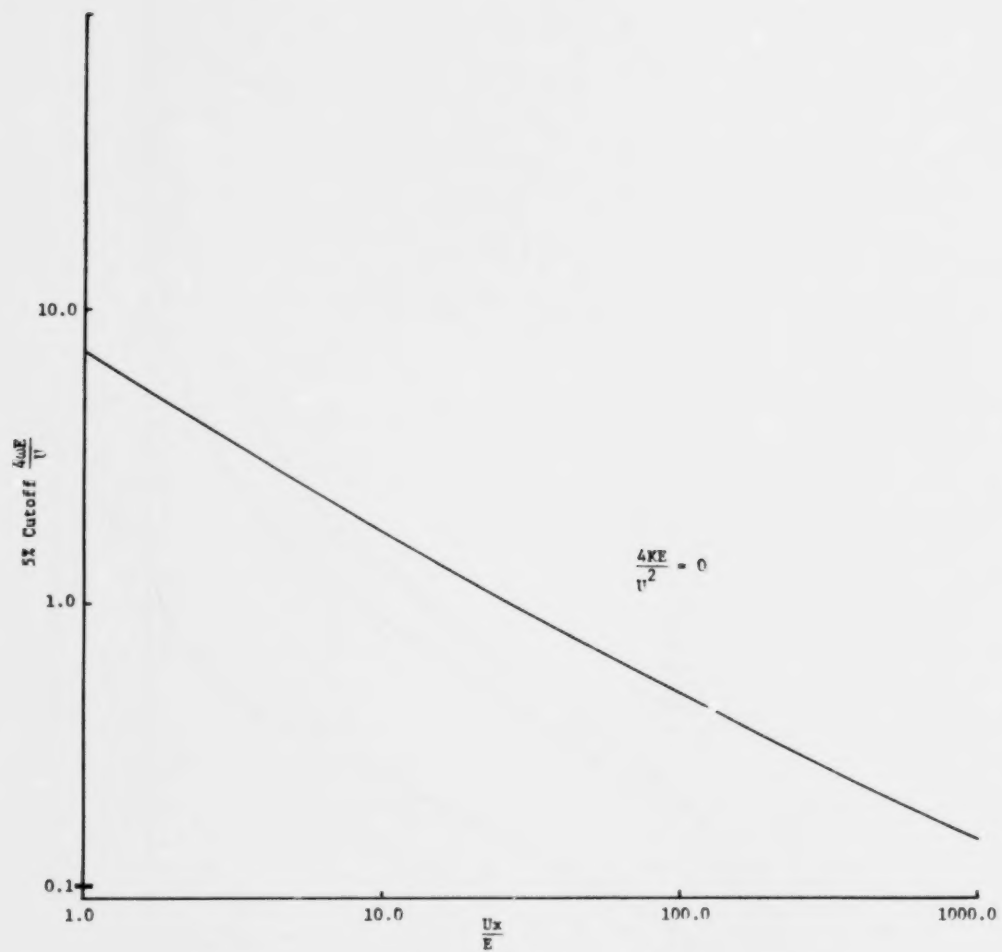


Figure 3.6 5% Cutoff with Zero Decay

level will be assumed. Aliasing phenomena are neglected in view of the arbitrary nature of the cutoff level. Practical experience will indicate which cutoff levels result in discretization Δx and Δt which are "just right". Figure 3.6 is a plot of the 5% cutoff $\frac{4\omega E}{U}$ versus dimensionless distance $\frac{Ux}{E}$ from the injection point. In a given problem, one can enter this plot and calculate

$$\omega_{\max} = \frac{U}{4E} \text{ (5\% cutoff)} \quad (3.50)$$

at various distances along the channel. The local network scale can be determined by substituting Equation (3.50) into Equation (3.45), and an estimate of the time step follows directly from Equations (3.44) and (3.46).

3.1.6 Tests of the Discretization Criteria

To test the discretization criteria and show how they are applied, two examples are considered. The first is the classical problem of propagation of a concentration front through a channel which is at zero initial concentration. The flow is at constant velocity and constant depth, and decay is neglected, so that the problem is described by the convective diffusion equation

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} = E \frac{\partial^2 c}{\partial x^2}, \quad 0 < x < \infty \quad (2.22)$$

The initial condition is

$$c(x, 0) = 0 \quad (3.51)$$

and the boundary conditions are

$$c(0, t) = 1.0, \quad t > 0 \quad (3.52a)$$

and

$$c(x,t) \rightarrow 0 \text{ as } x \rightarrow \infty, t > 0 \quad (3.52b)$$

The analytical solution for the concentration profile is

$$c = \frac{1}{2} \exp \left\{ \frac{Ux}{E} \right\} \operatorname{erfc} \left\{ \frac{x + Ut}{2 \sqrt{Et}} \right\} + \frac{1}{2} \operatorname{erfc} \left\{ \frac{x - Ut}{2 \sqrt{Et}} \right\} \quad (3.53)$$

In the numerical model, a downstream boundary must be taken at a finite distance from the origin. Therefore, boundary condition (3.52b) will not be applicable when the concentration front is in the vicinity of the downstream boundary. The situation, however, is analogous to the ocean boundary of an estuary where the concentration profile should pass out to sea in an unrestricted manner. Specifying the ebb formulation of the ocean boundary condition at the downstream boundary will be a useful test of its effect on concentration profiles.

Values of U and E are chosen which are typical of natural streams and estuaries:

$$U = 2.0 \frac{\text{ft}}{\text{sec}} \quad (3.54a)$$

and

$$E = 50 \frac{\text{ft}^2}{\text{sec}} \quad (3.54b)$$

With the parameters of Equations (3.54), the discretization criteria are:

$$\begin{aligned} \Delta x < \frac{1}{\omega_{\max}} &= \frac{4E}{U(5\% \text{ cutoff})} \\ &= \frac{100}{(5\% \text{ cutoff})} \end{aligned} \quad (3.55a)$$

$$\Delta t \leq \frac{\Delta x}{U} = \frac{\Delta x}{2} \quad (3.55b)$$

$$\Delta t \leq \frac{\Delta x^2}{2E} = \frac{\Delta x^2}{100} \quad (3.55c)$$

Table 3.1 shows the values of Δx and Δt calculated at various downstream points from Equations (3.55). The 5% cutoff is obtained from Figure 3.6. The results of Table 3.1 are consistent with what one might expect in trying to model the concentration profile from an instantaneous injection. At small distances, the profile is short and steep, requiring small Δx and Δt for good resolution. At larger distances, the profile broadens and flattens. It is interesting to note that for values of $\frac{Ux}{E} < 8$, dispersion governs the time step Δt . For values of $\frac{Ux}{E} > 8$, advection governs the time step.

Using the results of Table 3.1, a variable computational mesh is set up in Table 3.2. A time step Δt of 10 seconds is selected in order to handle the concentration profile accurately at small times and distances. Probably the time step could be increased as the profile moves downstream, but this was not considered worthwhile for practical purposes.

The results of the numerical computation are plotted in Figure 3.7 along with the analytical solution for the concentration profiles at selected times. The logarithmic distance scale distorts the profiles so that they appear to be steepening rather than flattening. Agreement is excellent, and there are no oscillations of the numerical solution, indicating good convergence. Of particular interest is the profile at

Table 3.1 Discretization Parameters for Propagation of a Steep Front

$x(\text{ft})$	$\frac{Ux}{B_E} = \frac{x}{25}$	(5% cutoff)	$\Delta x = \frac{100}{(5\% \text{ cutoff})}$	$\Delta t = \frac{\Delta x}{2} (\text{sec})$	$\Delta t = \frac{\Delta x^2}{100}$
50	2	4.74	21	10	4
100	4	3.08	32	16	10
200	8	2.00	50	25	25
500	20	1.18	85	42	72
1,000	40	.805	125	62	156
2,000	80	.559	180	90	324
5,000	200	.349	285	143	812
10,000	400	.246	405	203	1,640
20,000	800	.173	580	290	3,364

Table 3.2 Computational Mesh for Propagation of a Steep Front

Mesh Point	$\Delta x(\text{ft.})$	$x(\text{ft.})$	Mesh Point	$\Delta x(\text{ft.})$	$x(\text{ft.})$	Mesh Point	$\Delta x(\text{ft.})$	$x(\text{ft.})$
1		0	17	120	930	33	280	4210
2	25	25	18	130	1060	34	290	4500
3	25	50	19	140	1200	35	300	4800
4	25	75	20	150	1350	36	300	5100
5	25	100	21	160	1510	37	300	5400
6	30	130	22	170	1680	38	300	5700
7	35	165	23	180	1860	39	300	6000
8	40	205	24	190	2050	40	400	6400
9	45	250	25	200	2250	41	400	6800
10	50	300	26	210	2460	42	400	7200
11	60	360	27	220	2680	43	400	7600
12	70	430	28	230	2910	44	400	8000
13	80	510	29	240	3150	45	400	8400
14	90	600	30	250	3400	46	400	8800
15	100	700	31	260	3660	47	400	9200
16	110	810	32	270	3930	48	400	9600
						49	400	10000

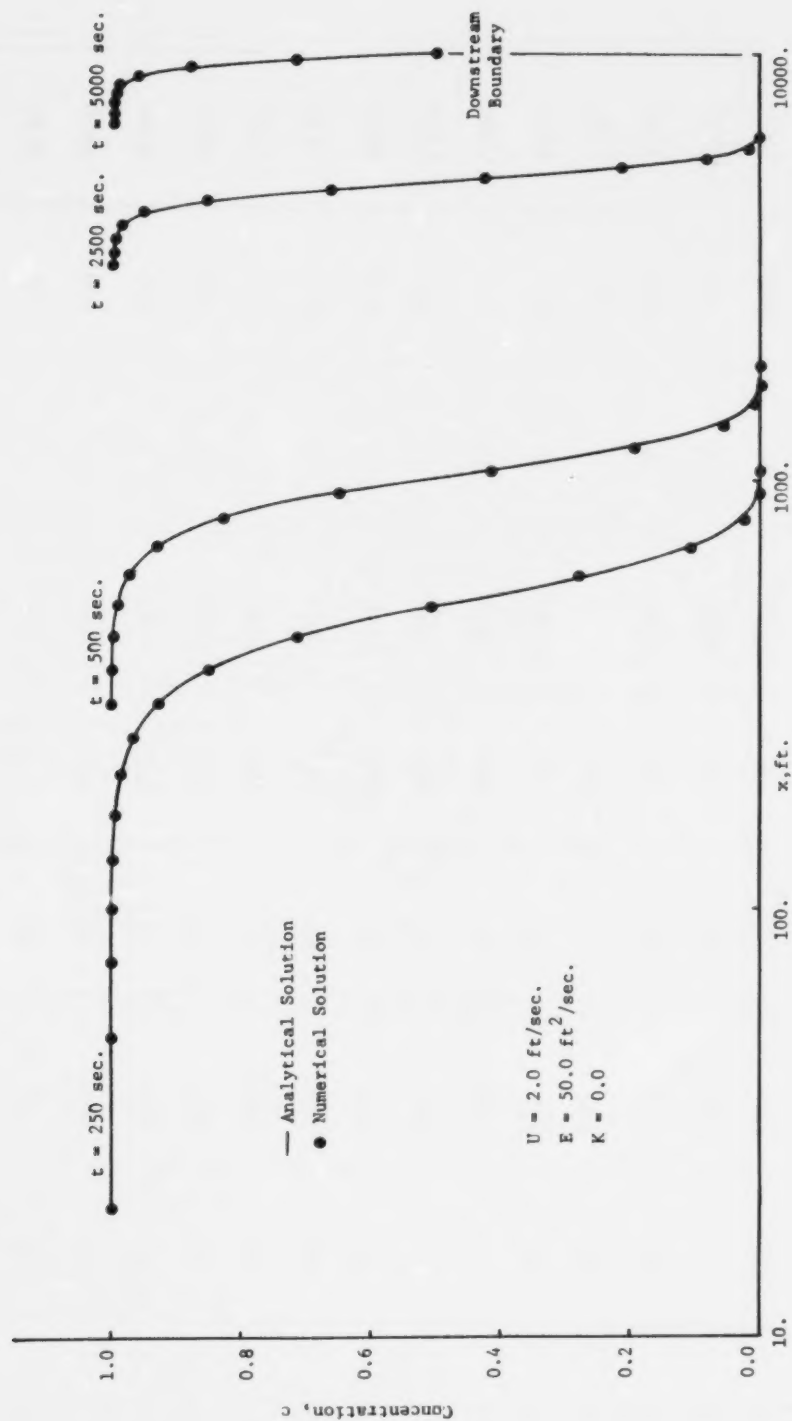


Figure 3.7 Propagation of a Steep Front

5000 seconds, which is in the midst of passing through the downstream boundary. The match of the analytical and computed results indicate that the ebb formulation of the ocean boundary condition will transmit a concentration profile with minimum distortion.

The second example considers the injection of non-conservative substance into a constant-area estuary with a simple harmonic tide. Assuming further that the dispersion coefficient is constant, the conservation of mass equation becomes:

$$\frac{\partial c}{\partial t} + \{U_f + U_T \sin \sigma(t - \theta_s)\} \frac{\partial c}{\partial x} = E \frac{\partial^2 c}{\partial x^2} - Kc \quad (3.55)$$

where

U_f = net advective flow velocity

U_T = amplitude of the tidal velocity

θ_s = time shift between the arbitrary time origin and the time of zero oscillating velocity at high water slack.

For the case of continuous injection beginning at $t = 0$, Harleman, Holley, and Huber (1966) have obtained an analytical solution for the concentration distribution in integral form:

$$\frac{c}{c_o} = \int_0^t \frac{U_f}{\sqrt{4\pi E(t-\tau)}} \exp \frac{-\{x - U_f(t-\tau) + \frac{U_T}{\sigma} (\cos \sigma t - \cos \sigma \tau)\}^2}{4E(t-\tau)} d\tau \quad (3.56)$$

where

$c_o = \frac{I}{\rho A U_f}$ = mixed concentration of injection and fresh water flow.

and

I = mass injection rate of substance

A = cross-sectional area of the estuary

A closed form solution of this integral is not known; however, it can be evaluated easily using numerical solution techniques.

For numerical computations, the coefficients in Equation (3.55) are assigned values which are identical to those used in an idealized channel study by Lee and Harleman (1971).

$$U_f = 0.1 \text{ ft/sec.}$$

$$U_T = 2.0 \text{ ft/sec.}$$

$$T = 44712 \text{ sec.}$$

(3.57)

$$E = 65 \text{ ft}^2/\text{sec.}$$

$$K = 0.034/\text{day}$$

These values might be typical of a prototype dye test in the fresh water tidal region of the Delaware estuary. In applying the discretization criteria, it is not clear what value should be chosen for the velocity U in the dimensionless distance parameter $\frac{Ux}{E}$. As a rule of thumb, it was decided to take U as the maximum tidal velocity and define Δx and Δt at one tidal excursion from the injection point. This Δx would then be imposed over one tidal excursion on either side of the injection point and Δt would be used as the solution time step.

It may be recalled that the spectral density of Equation (3.36), and hence the cutoff frequencies, is a function of the decay parameter $\frac{4KE}{U^2}$. The value of this parameter in this example is

$$\frac{4KE}{U^2} = 2.32 \times 10^{-5} \quad (3.58)$$

It was found that including this value in the calculation of cutoff frequencies caused an insignificant change in Figure 3.6. This is not too surprising if one looks at the exponential decay term in Equation (3.37) and observes that damping of higher harmonics in particular is dominated by dispersion rather than decay. Therefore, it is probably a reasonable and conservative assumption to ignore decay in applying the discretization criteria. The length of a tidal excursion is

$$\frac{UT}{\pi} \approx 30,000 \text{ ft.} \quad (3.59)$$

and the dimensionless distance parameter is

$$\frac{Ux}{E} \approx 970 \quad (3.60)$$

From Figure 3.6, the 5% cutoff is about 0.155. Therefore, the value of Δx can be calculated as

$$\begin{aligned} \Delta x &\leq \frac{4E}{U(5\% \text{ cutoff})} \\ &= 800 \text{ ft.} \text{.. say } 1000 \text{ ft.} \end{aligned} \quad (3.61)$$

and the time step will be

$$\Delta t \leq \frac{\Delta x}{U} \approx 500 \text{ seconds} \quad (3.62)$$

In their idealized channel study, Lee and Harleman observed that the concentration distribution far downstream of the injection point was very nearly that resulting from a non-tidal advective calculation. This is to be expected, since net movement of pollutant towards the sea

over a number of tidal cycles is controlled by fresh water throughflow. As an indication of the mesh spacing required far downstream, a calculation using the net advective flow velocity U_f was made near the downstream boundary.

$$U \rightarrow U_f = 0.1 \text{ ft/sec.}$$

$$\frac{Ux}{E} \approx \frac{0.1 \times 260,000}{65} = 400$$

$$(5\% \text{ cutoff}) = 0.245 \quad (\text{from Figure 3.6}) \quad (3.63)$$

$$\Delta x \leq \frac{4E}{U(5\% \text{ cutoff})}$$

$$\approx 10,000 \text{ ft.}$$

This estimate is quite conservative.

Figure 3.8 shows the results of a computation where Δx was specified as 1000 feet within a tidal excursion of the injection point. Downstream, Δx was gradually expanded to minimize the computations while maintaining good convergence. The time step Δt was selected as $\frac{T}{96} = 465.75$ seconds. Convergence of the numerical solution to the analytical solution is excellent, except for a ringing effect near the injection point. The ringing is caused by a discontinuity in the concentration gradient which the numerical solution finds hard to resolve. The effects on convergence of doubling Δx to 2000 feet are shown in Figure 3.9. Resolution of the concentration gradient near the injection point remains good, but the ringing effects are more pronounced. Sensitivity to the time step Δt is shown in Figure 3.10,

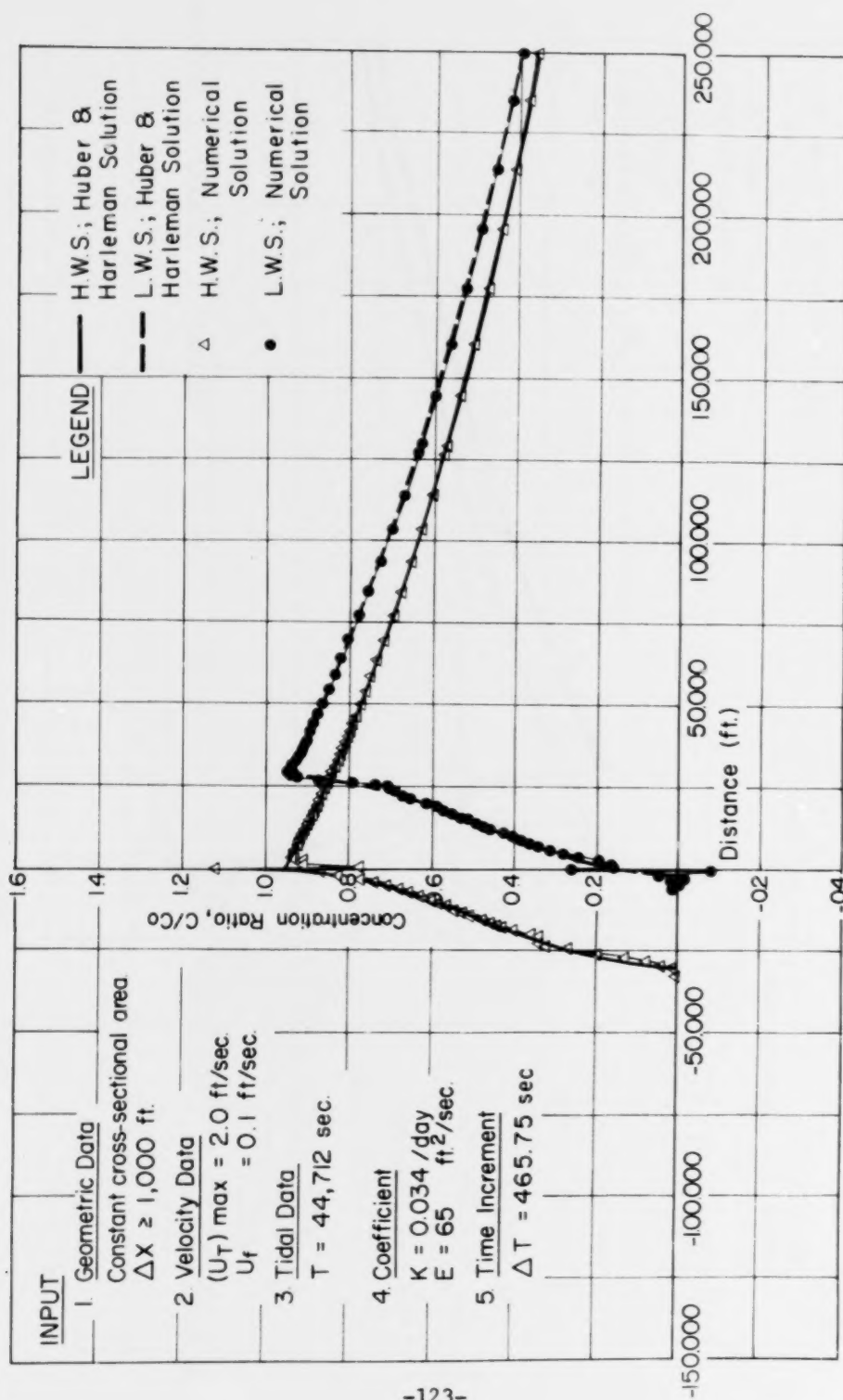


Figure 3.8 Comparison of Analytical Solution and Numerical Solution
with $\Delta x = 1000$ ft. and Greater and $\Delta t = 465.75$ sec.

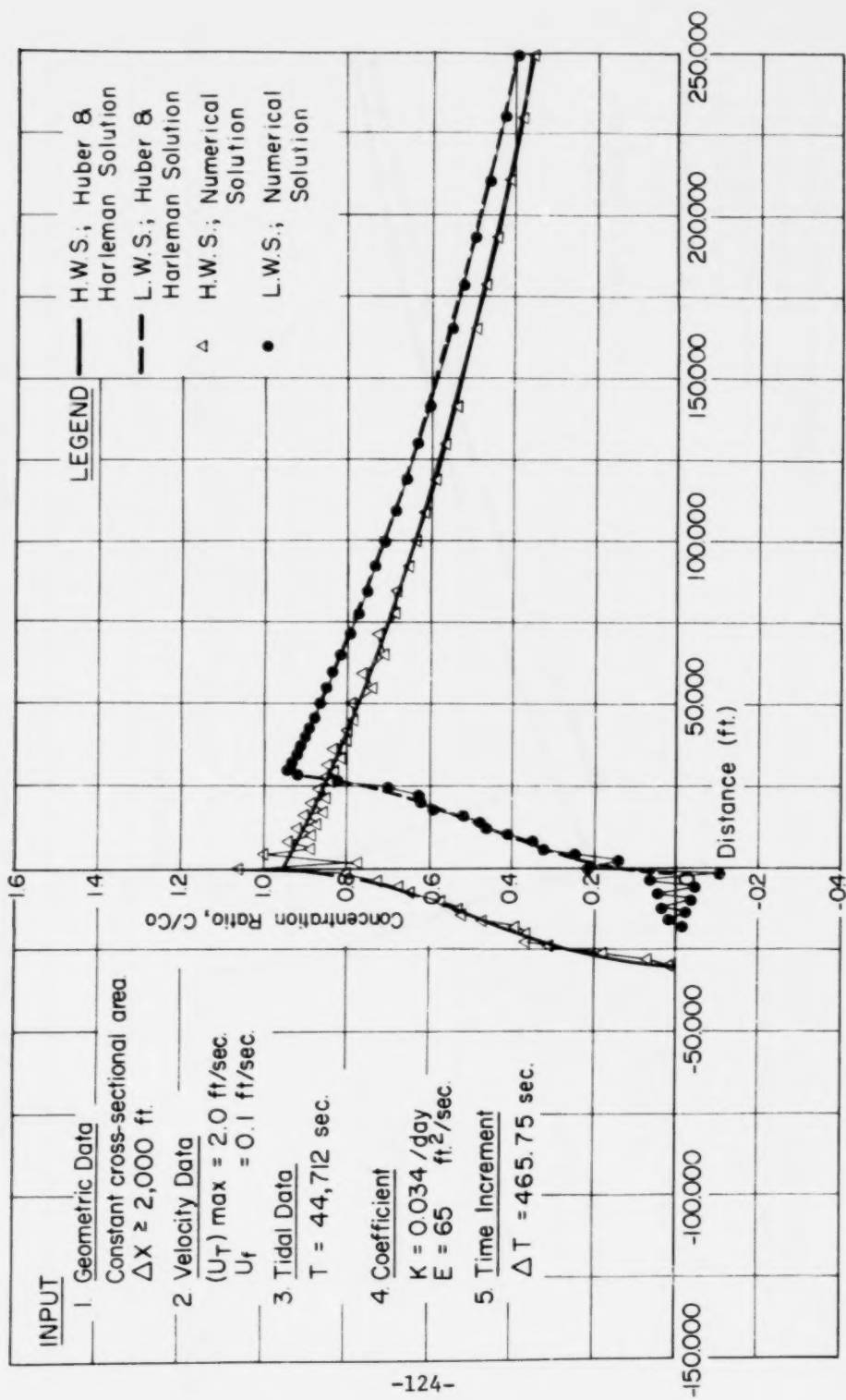


Figure 3.9 Effect of Increasing Δx to 2000 ft. and Greater

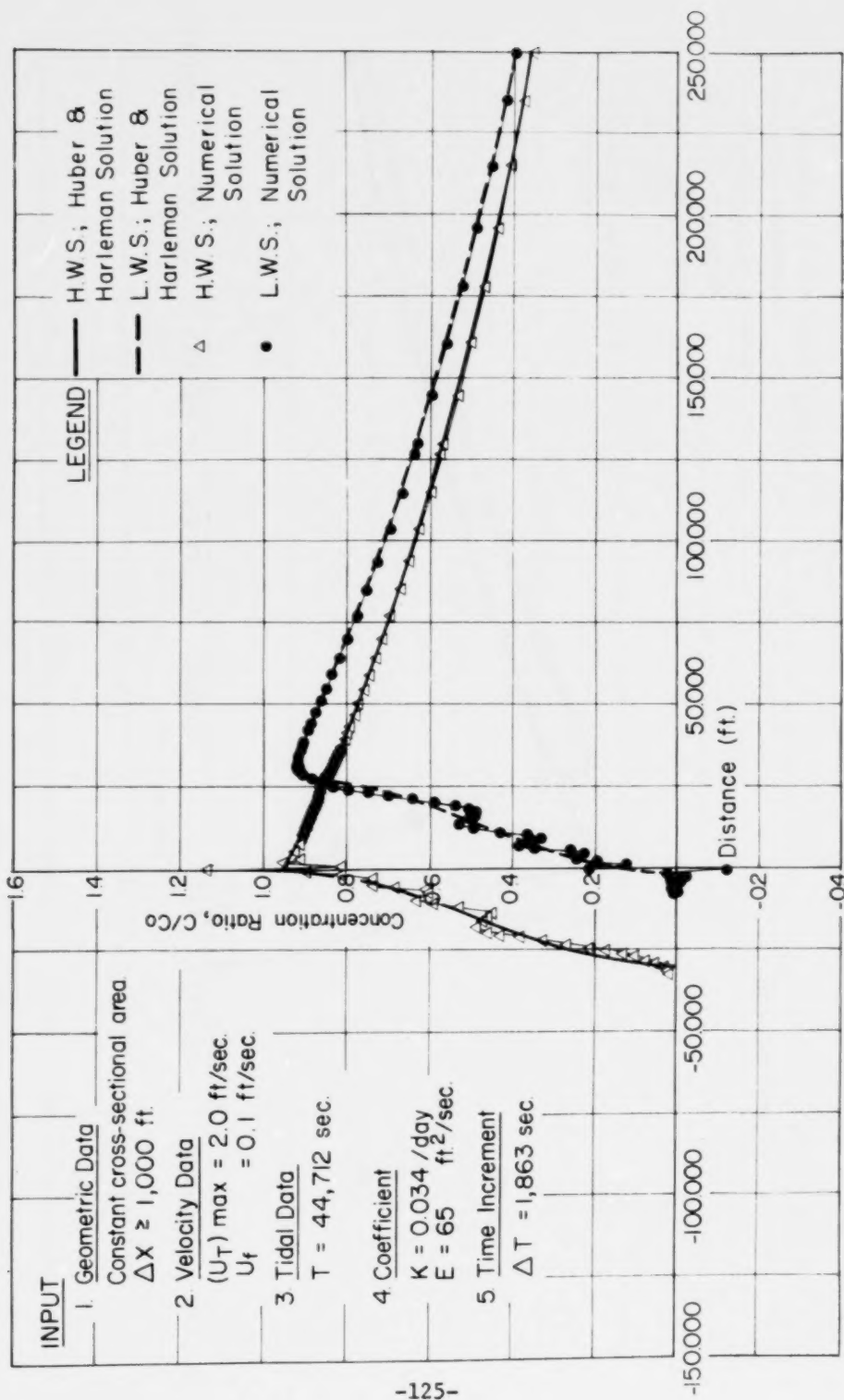


Figure 3.10 Effect of Increasing Δt to 1863 sec.

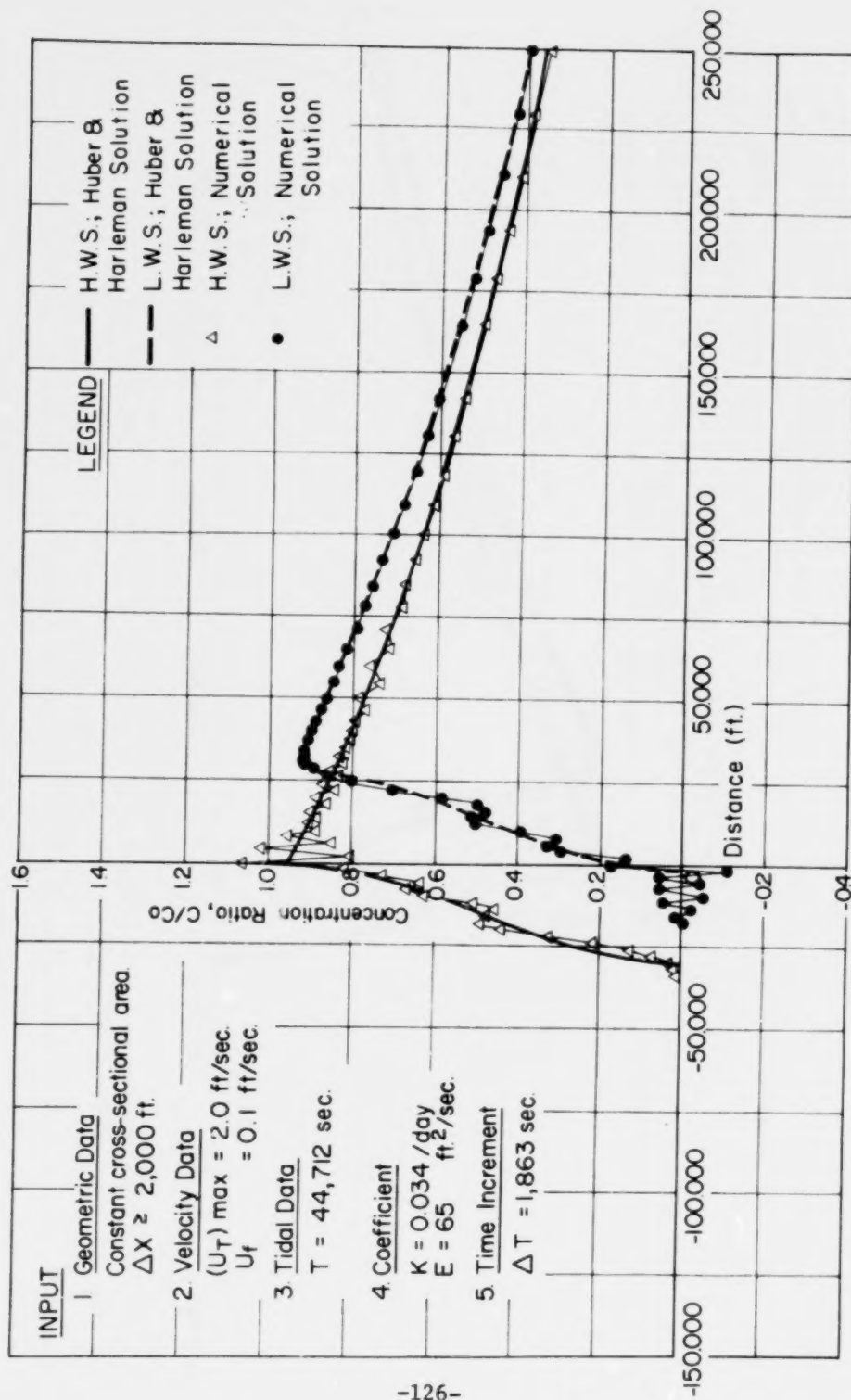


Figure 3.11 Effect of Increasing Δt to 1863 sec. and Δx to 2000 ft. and Greater

where Δx is 1000 feet and the time step has been quadrupled to 1863 seconds. Oscillations in the concentration gradient near the injection point have become more pronounced, indicating poorer convergence. Figure 3.11 shows the results of both quadrupling the time step and doubling Δx . As expected, convergence is the poorest of all.

It may be recalled that the analytic solution for this example is for an infinite channel. At the downstream boundary in the numerical computations, the ebb formulation of the ocean boundary condition is maintained over the entire tidal cycle. The resulting concentration profiles in Figures 3.8 through 3.11 match the analytic solution quite well.

3.2 Continuity and Momentum Equations

3.2.1 Finite Element, Implicit Scheme of Gunaratnum and Perkins

Gunaratnum and Perkins (1970) have developed a finite element, implicit technique for solving the St. Venant Equation in a network of channels. Their motivation in choosing this approach was the desire to minimize errors between the numerical scheme and the partial differential equations. As opposed to the work of Stone and Brian (1963) on the convective diffusion equation, it is very difficult to evaluate damping and phase factors both for the solution of the linearized form of the St. Venant Equations and for the numerical scheme. One means of assuring a "best fit" of the numerical solution to the exact, continuous solution is to apply the method of weighted residuals.

For the implicit solution procedure, Gunaratnum and Perkins cast the St. Venant Equations in characteristic form. It was felt that the

resulting set of simultaneous linear equations in the numerical scheme would be evenly balanced, making the numerical solution less susceptible to the effects of round-off in the computer. The characteristic form of the St. Venant Equations can be obtained in mathematically rigorous fashion by linear transformation. However, a very direct procedure is to multiply Equation (2.8) successively by $U + c$ and $U - c$ and subtract the results from Equation (2.17)

$$\begin{aligned} & \left(\frac{\partial z}{\partial t} + (U \pm c) \frac{\partial z}{\partial x} \right) - \frac{1}{B(U \mp c)} \left(\frac{\partial Q}{\partial t} + (U \pm c) \frac{\partial Q}{\partial x} \right) \\ &= - \frac{Ag}{B(U \mp c)} \left\{ \frac{F^2}{B} \frac{\partial A^2}{\partial x} - S_f - \frac{d}{\rho} \frac{\partial \rho}{\partial x} \right\} + \frac{q_L}{B} \end{aligned} \quad (3.64)$$

Equation (3.64) represents a pair of characteristic equations which include the effects of longitudinal density gradients.

To apply the method of weighted residuals, Equations (3.64) are linearized as follows.

$$\left(\frac{\partial z}{\partial t} + \lambda \frac{\partial z}{\partial x} \right) - \frac{1}{B_o \bar{\lambda}} \left(\frac{\partial Q}{\partial t} + \lambda \frac{\partial Q}{\partial x} \right) - \psi = 0 \quad (3.65)$$

where

$$\lambda = U \pm c \text{ (assumed constant)}$$

$$\bar{\lambda} = U \mp c \text{ (assumed constant)}$$

$$B_o = \text{constant topwidth}$$

$$\psi = - \frac{Ag}{B_o \bar{\lambda}} \left\{ \frac{F^2}{B} \frac{dA^2}{dx} - S_f - \frac{d}{\rho} \frac{\partial \rho}{\partial x} \right\} + \frac{q_L}{B} \text{ (assumed constant)}$$

Piecewise linear approximations of the water surface elevation z and the discharge Q are substituted into Equations (3.65) and the method of

weighted residuals is applied in the form of Galerkin's Method. The solution is propagated forward in time by assuming simple backward differences for the derivatives of water surface elevation and discharge at the mesh points:

$$\frac{dz_i}{dt} = \frac{z_i^{n+1} - z_i^n}{\Delta t} \quad (3.66a)$$

$$\frac{dQ_i}{dt} = \frac{Q_i^{n+1} - Q_i^n}{\Delta t} \quad (3.66b)$$

The quasi-linear nature of Equations (3.64) is reproduced in the numerical solution by updating the constant coefficients in Equations (3.65) at every time step. The first three coefficients become

$$\lambda \rightarrow \lambda_i^n = (U \pm c)_i^n \quad (3.67a)$$

$$\bar{\lambda} \rightarrow \bar{\lambda}_i^n = (U \mp c)_i^n \quad (3.67b)$$

$$B_o \rightarrow B_i^n \quad (3.67c)$$

The fourth coefficient Ψ receives a rather interesting treatment. It turns out that the friction slope S_f must be expanded in a Taylor series to make the implicit numerical scheme stable over a wide range of time steps Δt .

$$S_f^{t+\Delta t} = S_f^t + \frac{\partial S_f}{\partial z} \frac{\partial z}{\partial t} \Delta t + \frac{\partial S_f}{\partial Q} \frac{\partial Q}{\partial t} \Delta t \quad (3.68)$$

At a given mesh point i , Equation (3.68) can be written

$$\begin{aligned} \left(\frac{Q|Q|}{k^2}\right)_i^{n+1} &= \left(\frac{Q|Q|}{k^2}\right)_i^n - 2\left(\frac{Q|Q|}{k^2}\right)_i^n \left(\frac{1}{k} \frac{dk}{dz}\right)_i^n (z_i^{n+1} - z_i^n) \\ &+ \left(\frac{2|Q|}{k^2}\right)_i^n (Q_i^{n+1} - Q_i^n) \end{aligned} \quad (3.69)$$

where

$$k = A^2 C_z^2 R_h \quad (\text{a resistance coefficient})$$

The remaining terms in Ψ are updated in the same manner as the parameters in Equations (3.67)

Gunaratnum and Perkins use a uniform element size Δx over the length of a channel, so that the results of the method of weighted residuals resemble the results of a finite difference scheme. For each interior mesh point, the method of weighted residuals will yield a pair of equations for discrete water surface elevations and discharges.

$$a_1^i z_{i-1}^{n+1} + a_2^i Q_{i-1}^{n+1} + b_1^i z_i^{n+1} + b_2^i Q_i^{n+1} + c_1^i z_{i+1}^{n+1} + c_2^i Q_{i+1}^{n+1} = d_1^i \quad (3.70a)$$

$$a_3^i z_{i-1}^{n+1} + a_4^i Q_{i-1}^{n+1} + b_3^i z_i^{n+1} + b_4^i Q_i^{n+1} + c_3^i z_{i+1}^{n+1} + c_4^i Q_{i+1}^{n+1} = d_2^i \quad (3.70b)$$

where

$$a_1^i = \frac{1}{6} - \frac{\lambda_1^{i,n}}{2} \frac{\Delta t}{\Delta x}$$

$$a_2^i = \frac{-1}{B_i^n \lambda_2^{i,n}} a_1^i$$

$$a_3^i = \frac{1}{6} - \frac{\lambda_2^{i,n}}{2} \frac{\Delta t}{\Delta x}$$

$$a_4^i = \frac{-1}{B_i^n \lambda_1^{i,n}} a_3^i$$

$$b_1^i = \frac{2}{3} + 2\Delta t \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_i^n \left(\frac{Ag}{B\lambda_2} \right)_i^n$$

$$b_2^i = \frac{1}{-B_i^n \lambda_2^{i,n}} \left(\frac{2}{3} + 2\Delta t \left(Ag \frac{|Q|}{k^2} \right)_i^n \right)$$

$$b_3^i = \frac{2}{3} + 2\Delta t \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_i^n \left(\frac{Ag}{B\lambda_1} \right)_i^n$$

$$b_4^i = - \frac{1}{B_i^n \lambda_1^{i,n}} \left(\frac{2}{3} + 2\Delta t \left(Ag \frac{|Q|}{k^2} \right)_i^n \right)$$

$$c_1^i = \frac{1}{6} + \frac{\lambda_1^{i,n}}{2} \frac{\Delta t}{\Delta x}$$

$$c_2^i = \frac{-1}{B_i^n \lambda_2^{i,n}} c_1^i$$

$$c_3^i = \frac{1}{6} + \frac{\lambda_2^{i,n}}{2} \frac{\Delta t}{\Delta x}$$

$$c_4^i = \frac{-1}{B_i^n \lambda_1^{i,n}} c_3^i$$

$$d_1^i = - \Delta t \left(\frac{Ag}{B\lambda_2} \right)_i^n \left[\left(\frac{F^2}{B} \frac{\partial A^z}{\partial x} \right)_i^n + \left(\frac{Q|Q|}{k^2} \right)_i^n - 2 \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_i^n z_i^n - \left(\frac{d}{\rho} \frac{\partial \rho}{\partial x} \right)_i^n \right]$$

$$+ \frac{q_{L,i}^{n+1} \Delta t}{B_i^n} + \left(\frac{1}{6} z_{i-1}^n + \frac{2}{3} z_i^n + \frac{1}{6} z_{i+1}^n \right)$$

$$- \frac{1}{B_i^n \lambda_2^{i,n}} \left(\frac{1}{6} Q_{i-1}^n + \frac{2}{3} Q_i^n + \frac{1}{6} Q_{i+1}^n \right)$$

$$d_2^i = - \Delta t \left(\frac{Ag}{B\lambda_1} \right)_i^n \left[\left(\frac{F^2}{B} \frac{\partial A^z}{\partial x} \right)_i^n + \left(\frac{Q|Q|}{k^2} \right)_i^n - 2 \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_i^n z_i^n - \left(\frac{d}{\rho} \frac{\partial \rho}{\partial x} \right)_i^n \right]$$

$$+ \frac{q_{L,i}^{n+1} \Delta t}{B_i^n} + \left(\frac{1}{6} z_{i-1}^n + \frac{2}{3} z_i^n + \frac{1}{6} z_{i+1}^n \right)$$

$$- \frac{1}{B_i^n \lambda_1^{i,n}} \left(\frac{1}{6} Q_{i-1}^n + \frac{2}{3} Q_i^n + \frac{1}{6} Q_{i+1}^n \right)$$

and

$$\lambda_1^{i,n} = (U + c)_i^n$$

$$\lambda_2^{i,n} = (U - c)_i^n$$

At the boundary mesh points either water surface elevation or discharge will be prescribed. Therefore, only one additional equation for the remaining variable will be required at each boundary. At the upstream

boundary, the equation for the backward characteristic in the first element Δx is the appropriate choice. This equation is:

$$b_3^1 z_1^{n+1} + b_4^1 Q_1^{n+1} + c_3^1 z_2^{n+1} + c_4^1 Q_2^{n+1} = d_2^1 \quad (3.70c)$$

where

$$b_3^1 = \frac{1}{3} + \Delta t \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_1^n \left(\frac{Ag}{B\lambda_1} \right)_1^n$$

$$b_4^1 = - \frac{1}{B_1^n \lambda_1^{1,n}} \left(\frac{1}{3} + \Delta t \left(Ag \frac{|Q|}{k^2} \right)_1^n \right)$$

$$c_3^1 = \frac{1}{6} + \frac{\lambda_2^{1,n}}{2} \frac{\Delta t}{\Delta x}$$

$$c_4^1 = - \frac{1}{B_1^n \lambda_1^{1,n}} c_3^1$$

$$d_2^1 = - \frac{\Delta t}{2} \left(\frac{Ag}{B\lambda_1} \right)_1^n \left[\left(\frac{F^2}{B} \frac{\partial A^z}{\partial x} \right)_1^n + \left(\frac{Q|Q|}{k^2} \right)_1^n - 2 \left(\frac{Q|Q|}{k^3} \frac{dk}{dz} \right)_1^n z_1^n - \left(\frac{d}{\rho} \frac{\partial \rho}{\partial x} \right)_1^n \right]$$

$$+ \frac{q_{L,1}^{n+1} \Delta t}{2B_1^n} + \left(\frac{1}{3} z_1^n + \frac{1}{6} z_2^n \right)$$

$$- \frac{1}{B_1^n \lambda_1^{1,n}} \left(\frac{1}{3} Q_1^n + \frac{1}{6} Q_2^n \right)$$

At the downstream boundary, the forward characteristic in the last element Δx is taken, yielding the equation:

$$a_1^N z_{N-1}^{n+1} + a_2^N Q_{N-1}^{n+1} + b_1^N z_N^{n+1} + b_2^N Q_N^{n+1} = d_1^N \quad (3.70)$$

where

$$a_1^N = \frac{1}{6} - \frac{\lambda_1^{N,n}}{2} \frac{\Delta t}{\Delta x}$$

$$a_2^N = \frac{-1}{B_N^n \lambda_2^{N,n}} a_1^N$$

$$b_1^N = \frac{1}{3} + \Delta t \left(\frac{Q|Q|}{3k} \frac{dk}{dz} \right)_N^n \left(\frac{Ag}{B\lambda_2} \right)_N^n$$

$$b_2^N = - \frac{1}{B_N^n \lambda_2^{N,n}} \left(\frac{1}{3} + \Delta t \left(Ag \frac{|Q|}{k^2} \right)_N^n \right)$$

$$d_1^N = - \frac{\Delta t}{2} \left(\frac{Ag}{B\lambda_2} \right)_N^n \left[\left(\frac{F^2}{B} \frac{\partial A^z}{\partial x} \right)_N^n + \left(\frac{Q|Q|}{k^2} \right)_N^n - 2 \left(\frac{Q|Q|}{3k} \frac{dk}{dz} \right)_N^n z_N^n - \left(\frac{dc}{\rho} \frac{\partial \rho}{\partial x} \right)_N^n \right]$$

$$+ \frac{q_{L,N}^{n+1} \Delta t}{2B_N^n} + \left(\frac{1}{6} z_{N-1}^n + \frac{1}{3} z_N^n \right)$$

$$- \frac{1}{B_N^n \lambda_2^{N,n}} \left(\frac{1}{6} Q_{N-1}^n + \frac{1}{3} Q_N^n \right)$$

and

N = number of hydraulic mesh points in the channel.

The $2N-2$ equations represented by Equation (3.70) and 2 boundary conditions are sufficient to determine the $2N$ values of z_i and Q_i . Equation (3.70) may be written in matrix form as:

$$\underline{A} \underline{x} = \underline{d} \quad (3.71)$$

where

$$\underline{\underline{A}} =$$

$$\underline{x} = \begin{bmatrix} z_1 \\ Q_1 \\ z_2 \\ Q_2 \\ \vdots \\ z_{N-1} \\ Q_{N-1} \\ z_N \\ Q_N \end{bmatrix} \quad \underline{d} = \begin{bmatrix} d_2^1 \\ d_1^2 \\ d_2^2 \\ \vdots \\ d_1^{N-1} \\ d_2^{N-1} \\ d_1^N \end{bmatrix}$$

The procedure for solving this set of equations in the context of a channel network will be discussed in section 4.3. However, it may be noted here that the submatrix in $\underline{A}$ which is contained within the dashed lines is bitridiagonal in nature. This means that the set of equations for the interior mesh points can be solved by a very efficient computational procedure.

3.2.2 Initial Condition and Boundary Conditions

To start off the computations, it is necessary to supply initial estimates of the water surface elevation z_1^1 and the discharges Q_1^1 . Usually,

the initial conditions are not known, and for practical purposes they need not be. In tidal hydraulics computations, it is common practice to make a very crude estimate of the initial conditions and then run the computations for a few tidal cycles prior to the period of interest. This way, the starting transient has time to die out, and computations "forget" what the initial condition was. The number of tidal cycles required will depend on the particular estuary, but ordinarily, it is five or less.

Specification of boundary conditions in tidal hydraulics computations is fairly straightforward. At an ocean boundary, a tide curve of water surface elevation versus time is prescribed. Often, this takes the form of a sinusoid with a range taken from the U.S.C. and G.S. Tide Tables. Upstream boundaries take one of two forms. At a head of tide such as a fall line or a dam, longitudinal transport of momentum through the boundary is zero. Therefore, the discharge is specified as zero, and fresh water inflow is entered as a lateral inflow. If there is no head of tide, the upstream boundary may be extended beyond the expected region of tidal motion to a point where river discharge can be prescribed with confidence.

3.2.3 Discretization Criteria

Gunaratnum and Perkins performed an approximate analysis of the numerical scheme and proposed the following criteria:

$$\frac{L}{\Delta x} \geq 100 \quad (3.72a)$$

$$\frac{\Delta t}{\Delta x} (U_o + c_o) \leq 5.5 \quad (3.72b)$$

where

L = shortest significant wave length

U_o = linearized velocity

c_o = linearized wave celerity

Estimation of the parameter L is based on an average streamflow friction slope which is difficult to evaluate in tidal flows. Even if an estimate were easily obtained, it would probably be overly conservative since the discretization criteria are based on a unit impulse, and tidal flows vary quite slowly in time. In practical applications, the choice of Δx is often governed by physical constraints. A short channel in a network will require two or three interior mesh points, placing an upper limit on Δx . Also, highly irregular channels may require a fine mesh to obtain a smooth numerical solution. However, the mesh must not be so fine as to consume excessive amounts of computer time.

Wood, Harley and Perkins (1972) have found that under certain conditions, Equations (3.72) may not be sufficiently stringent. This investigation was motivated by difficulties which were experienced in computing flows in shallow, highly irregular channels.

CHAPTER IV
PROGRAMMING CONSIDERATIONS

4.1 Network Formulation

For efficient execution on the computer, the network solution procedure should be straightforward and mechanical, with a minimum of bookkeeping and complex decision making. Certain programming languages such as FORTRAN execute arithmetic instructions very quickly, but they execute logical instructions slowly. With the goal of simplicity in mind, the first step in formulating the network solution procedure is definition of the network topology. To show how this is done, consider Figure 4.1, which might represent flow around an island. This network includes considerations which arise both in tree-like networks and networks which contain loops.

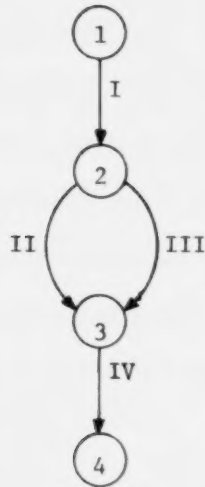


Figure 4.1 Example Network

For later use, the channels in a network will be termed "reaches" and the channel intersections will be termed "nodes". Using these definitions, the connectivity of the example network is defined in Table 4.1.

Table 4.1 Connectivity of Example Network

Reach	Upstream Node	Downstream Node
I	1	2
II	2	3
III	2	3
IV	3	4

The descriptions "upstream node" and "downstream node" in Table 4.1 have meaning only in the context that they provide a sign convention for the coordinate system in a reach. Positive direction x implies positive discharge Q . In an estuary, the ocean boundary could be taken at either node 1 or node 4 as long as the sign conventions within the reaches remain consistent. Auxiliary tables for convenient reference in the computations may be derived from Table 4.1, however, they will not be discussed here.

4.2 Method of Superposition

A basic technique in formulating the network solution procedure is the method of superposition, which was proposed for channel network

computations by Gunarantun and Perkins (1970). It resembles the method of influence functions which is commonly used in structural analysis. The technique makes use of the fact that, at a given time step, the solutions for water surface elevations, discharges, and concentrations at mesh points are given by sets of simultaneous linear equations. Because these equations are linear the principle of superposition will hold. The actual mechanics of executing the method of superposition are discussed in the following section; however, the basic notions are simple. In a given reach, the solution may be decoupled from the boundary mesh points by solving a set of equations for the interior mesh points under the assumption that solution values at the boundary mesh points are zero. This will be called a null solution. Using the same set of equations, influence factors due to unit solution values at the boundary mesh points are computed at the interior mesh points. There remains a set of equations for the boundary mesh points, which may be solved after the boundary conditions are included. Solution values at the interior mesh points are obtained next by multiplying the boundary solution values by the influence factors and adding the products to the null solution.

4.3 Solution Procedure for Water Surface Elevations and Discharges

In line with the operational features of the method of superposition, discussion of the solution procedure will be divided into two sections; one on interior mesh points and the other on boundary mesh points. Section 4.3.1, interior mesh points, is taken from the work of Gunarantun and Perkins. The rudiments of section 4.3.2 on boundary mesh points

are from the work of Wood, Harley and Perkins (1972); however, the actual procedure discussed is a result of the present study.

4.3.1 Interior Mesh Points

The notation in this section is taken directly from Gunaratnum and Perkins (1970). It differs from the notation used previously in that it is adjusted to conform more closely with subscripted variable notation in FORTRAN programming. The time step superscript $n+1$ has been dropped from water surface elevations and discharges.

At mesh point j , the water surface elevation $z(j)$ and the discharge $Q(j)$ may be written in terms of their respective null solutions and products of the appropriate influence factors and boundary values:

$$z(j) = z^0(j) + dx_1(j) \cdot z(1) + dx_3(j) \cdot Q(1) + dx_{11}(j) \cdot z(N) + dx_{33}(j) \cdot Q(N) \quad (4.1a)$$

$$Q(j) = Q^0(j) + dx_2(j) \cdot z(1) + dx_4(j) \cdot Q(1) + dx_{22}(j) \cdot z(N) + dx_{44}(j) \cdot Q(N) \quad (4.1b)$$

where

$z^0(j)$ = null solution for $z(j)$

$dx_1(j)$ = influence on $z(j)$ of unit $z(1)$

$dx_3(j)$ = influence on $z(j)$ of unit $Q(1)$

$dx_{11}(j)$ = influence on $z(j)$ of unit $z(N)$

$dx_{33}(j)$ = influence on $z(j)$ of unit $Q(N)$

$Q^0(j)$ = null solution for $Q(j)$

$dx_2(j)$ = influence on $Q(j)$ of unit $z(1)$

$dx_4(j)$ = influence on $Q(j)$ of unit $Q(1)$

$dx_{22}(j)$ = influence on $Q(j)$ of unit $z(N)$

$dx_{44}(j)$ = influence on $Q(j)$ of unit $Q(N)$

The null solution and the influence coefficients may be obtained in a single operation by solving the following matrix equation in the computer.

$$\underline{\underline{A}}' \underline{\underline{x}}' = \underline{\underline{d}}' \quad (4.2)$$

where

$\underline{\underline{A}}'$ = the $2N-4 \times 2N-4$ bitridiagonal submatrix which is defined by the dashed lines in the coefficient matrix $\underline{\underline{A}}$ of Equation (3.71).

$$\underline{\underline{x}}' = \begin{bmatrix} z^0(2) & dx_1(2) & dx_3(2) & dx_{11}(2) & dx_{33}(2) \\ Q^0(2) & dx_2(2) & dx_4(2) & dx_{22}(2) & dx_{44}(2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ z^0(N-1) & dx_1(N-1) & dx_3(N-1) & dx_{11}(N-1) & dx_{33}(N-1) \\ Q^0(N-1) & dx_2(N-1) & dx_4(N-1) & dx_{22}(N-1) & dx_{44}(N-1) \end{bmatrix}$$

$$\underline{\underline{d}}' = \begin{bmatrix} d_1^2 & -a_1^2 & -a_2^2 & 0 & 0 \\ d_2^2 & -a_3^2 & -a_4^2 & \vdots & \vdots \\ \vdots & 0 & 0 & 0 & 0 \\ d_1^{N-1} & \vdots & \vdots & -c_1^{N-1} & -c_2^{N-1} \\ d_2^{N-1} & 0 & 0 & -c_3^{N-1} & -c_4^{N-1} \end{bmatrix}$$

The first column of $\underline{d}'$ supplies the null solution when water surface elevation and discharge are prescribed as zero at the upstream and downstream boundaries. The remaining four columns in $\underline{d}'$ are the carry-overs from the appropriate columns outside the dashed lines in matrix $\underline{A}$ of Equation (3.71). When unit water surface elevations and discharges are prescribed at the boundaries, the appropriate columns in $\underline{A}$ are multiplied by 1 and moved to vectors in $\underline{d}'$.

A double sweep algorithm for solving a set of simultaneous linear equations whose coefficient matrix is bitridiagonal is given by Gunaratnum and Perkins. The five solution vectors in $\underline{x}'$ are obtained by generalizing this algorithm to handle five right-hand sides. Since the solution procedure is essentially Gauss reduction, the coefficient matrix must be decomposed only once rather than five times.

Once the boundary values are computed, as shown in the following section, $z(j)$ and $Q(j)$ may be determined by back-substitution.

4.3.2 Boundary Mesh Points

From Equation (3.71), the first and last equations remain to be used in solving for the boundary values. These equations may be written in terms of only the boundary values by replacing $z(2)$, $Q(2)$, $z(N-1)$ and $Q(N-1)$ with Equation (4.1)

$$\alpha_1 z(1) + \alpha_2 Q(1) + \alpha_3 z(N) + \alpha_4 Q(N) = D_2^1 \quad (4.3a)$$

$$\beta_1 z(1) + \beta_2 Q(1) + \beta_3 z(N) + \beta_4 Q(N) = D_1^N \quad (4.3b)$$

where

$$\alpha_1 = b_3(1) + dx_1(2) \cdot c_3(1) + dx_2(2) \cdot c_4(1)$$

$$\alpha_2 = b_4(1) + dx_3(2) \cdot c_3(1) + dx_4(2) \cdot c_4(1)$$

$$\alpha_3 = dx_{22}(2) \cdot c_3(1) + dx_{22}(2) \cdot c_4(1)$$

$$\alpha_4 = dx_{33}(2) \cdot c_3(1) + dx_{44}(2) \cdot c_4(1)$$

$$\beta_1 = dx_1(N-1) \cdot a_1(N) + dx_2(N-1) \cdot a_2(N)$$

$$\beta_2 = dx_3(N-1) \cdot a_1(N) + dx_4(N-1) \cdot a_2(N)$$

$$\beta_3 = b_1(N) + dx_{11}(N-1) \cdot a_1(N) + dx_{22}(N-1) \cdot a_2(N)$$

$$\beta_4 = b_2(N) + dx_{33}(N-1) \cdot a_1(N) + dx_{44}(N-1) \cdot a_2(N)$$

$$D_2^1 = d_2^1 - c_3(1) \cdot z^0(2) - c_4(1) \cdot Q^0(2)$$

$$D_1^N = d_1^N - a_1(N) \cdot z^0(N-1) - a_2(N) \cdot Q^0(N-1)$$

Equations (4.3) and two boundary conditions are sufficient to solve for the water surface elevations and discharges at the boundary mesh points. In formulating the network solution procedure it is useful to consider the example network in Figure 4.1 once again. For each reach that enters a node, the boundary water surface elevation and the boundary discharge are unknown. As an example, there are 6 unknowns at node 2. To solve for these unknowns there is one boundary equation for each reach which enters the node. The remaining equations must be specified by boundary conditions. Thus, at exterior nodes 1 and 4,

a single boundary condition specifying water surface elevation or discharge is required. At interior nodes 2 and 3, the required boundary conditions are supplied by compatibility of water surface elevations and continuity of discharge. Returning to node 2, the compatibility condition is

$$z_N^I = z_1^{II} = z_1^{III} \quad (4.4)$$

where

z_N^I = water surface elevation at mesh point N of reach I

z_1^{II} = water surface elevation at mesh point 1 of reach II

z_1^{III} = water surface elevation at mesh point 1 of reach III

and the continuity condition is

$$Q_N^I - Q_1^{II} - Q_1^{III} = 0 \quad (4.5)$$

where

Q_N^I = discharge at mesh point N of reach I

Q_N^{II} = discharge at mesh point 1 of reach II

Q_1^{III} = discharge at mesh point 1 of reach III

The equations are grouped for solution by looping over the nodes. At each node, the compatibility condition is enforced by solving for a single water surface elevation. Then the boundary equations offset the unknown discharges which enter the node, and either a boundary condition or a continuity condition offsets the water surface elevation. In matrix form, the set of equations for the boundary values of the

example network are grouped as follows:

α_1^I	α_2^I	α_3^I	α_4^I			z_1	$D_2^{1,I}$
1						Q_1^I	$\bar{z}$
β_1^I	β_2^I	β_3^I	β_4^I			z_2	$D_1^{N,I}$
		α_1^{II}	α_2^{II}	α_3^{II}	α_4^{II}	Q_N^I	$D_2^{1,II}$
		α_1^{III}	α_2^{III}	α_3^{III}	α_4^{III}	Q_1^{II}	$D_2^{1,III}$
			1	-1	-1	Q_1^{III}	0
	β_1^{II}	β_2^{II}	β_3^{II}	β_4^{II}		z_3	$D_1^{N,II}$
	β_1^{III}	β_2^{III}	β_3^{III}	β_4^{III}		Q_N^{II}	$D_1^{N,III}$
			α_1^{IV}	α_2^{IV}	α_3^{IV}	α_4^{IV}	$D_2^{1,IV}$
				1	1	-1	0
			β_1^{IV}	β_2^{IV}	β_3^{IV}	β_4^{IV}	$D_1^{N,IV}$
						1	$\bar{Q}$
						Q_N^{IV}	

(4.6)

In Equation (4.6) water surface elevation $\bar{z}$ is specified at node 1 and discharge $\bar{Q}$ is specified at node 4.

A very fortunate result of grouping the equations in this way is that the coefficient matrix of Equation (4.6) is banded. The bandwidth can be determined by checking each reach and looking for the maximum throws of the nodal submatrices from the main diagonal. In large networks, the banded structure of the coefficient matrix becomes very important computationally. The number of unknowns being evaluated in Equations (4.6) is twice the number of reaches plus the number of nodes. For a network of 30 reaches and 30 nodes, the coefficient matrix will be 90×90 , requiring more than 32^K bytes of computer storage in standard precision. Depending on the network topology and efficient node numbering, banding may significantly reduce the core storage requirements and improve execution times.

4.4 Solution Procedure for Concentrations

Formulation of the network solution procedure for concentrations parallels that for hydraulics. In the following two sections, discussion is limited to a single constituent. However, procedures developed for a single constituent can be used repetitively for a set of multiple constituents where interactions are sequential. This is the case for the four constituent sequence of salinity, temperature, BOD, and DO. In the case where constituents interact arbitrarily, the solution procedure can probably be generalized without too much difficulty to handle multiple constituents simultaneously.

4.4.1 Interior Mesh Points

Referring to Equation (3.17) the set of equations defining the mesh point concentrations in a reach may be written in more compact form as:

$$\left[\begin{array}{cc|c} a(1) & c(1) & \\ \hline b(2) & a(2) & c(2) \\ & \diagdown & \diagup \\ & \diagup & \diagdown \\ & b(M-1) & a(M-1) \\ & \diagup & \diagdown \\ & b(M) & a(M) \end{array} \right] \left[\begin{array}{c} \bar{c}(1) \\ \hline \bar{c}(2) \\ \vdots \\ \hline \bar{c}(M-1) \\ \hline \bar{c}(M) \end{array} \right]^{n+1} = \left[\begin{array}{c} \eta_1 \Delta t + B_1 \\ \hline B_2 \\ \vdots \\ \hline B_{M-1} \\ \hline \eta_M \Delta t + B_M \end{array} \right] \quad (4.7)$$

where

$$B_1 = d_a^{1-n} c_1^{-n} + d_c^{1-n} c_2^{-n} + (\text{source terms})_1$$

$$B_i = d_{B,j-1}^{1-n} + d_{a,j}^{1-n} + d_{c,j+1}^{1-n} + (\text{source terms})_i, \quad 2 \leq j \leq M-1$$

$$B_M = d_{B \cdot c}^{M-n} B_{M-1} + d_a^{M-n} + (\text{source terms})_M$$

As in the hydraulics, the notation is modified somewhat to conform more closely with subscripted variable notation in FORTRAN programming.

The method of superposition is applied by writing the mesh point concentrations in terms of their respective null solutions and products of the appropriate influence factors and boundary values.

$$\bar{c}(j) = \bar{c}^0(j) + \bar{c}(1) \cdot dx_1(j) + \bar{c}(M) \cdot dx_M(j) \quad (4.8)$$

where

$$\bar{c}^0(j) = \text{null solution for } \bar{c}(j)$$

$$dx_1(j) = \text{influence on } \bar{c}(j) \text{ of unit } \bar{c}(1)$$

$$dx_M(j) = \text{influence on } \bar{c}(j) \text{ of unit } \bar{c}(M)$$

The null solutions and influence coefficients are computed by considering all but the first and last of Equations (4.7).

$$\underline{\underline{A'}} \underline{\underline{x'}} = \underline{\underline{B'}} \quad (4.9)$$

where

$\underline{\underline{A'}}$ = the $M-2 \times M-2$ tridiagonal submatrix within the dashed lines of the coefficient matrix in Equations (4.7)

$$\underline{\underline{x'}} = \begin{bmatrix} \bar{c}^0(2) & dx_1(2) & dx_M(2) \\ | & | & | \\ | & | & | \\ | & | & | \\ | & | & | \\ \bar{c}^0(M-1) & dx_1(M-1) & dx_M(M-1) \end{bmatrix}$$

$$\underline{\underline{B'}} = \begin{bmatrix} B_2 & -b(2) & 0 \\ | & | & | \\ | & | & | \\ | & | & | \\ | & | & | \\ B_{M-1} & 0 & -c(2) \end{bmatrix}$$

As in the hydraulics, the first column of $\underline{B}'$ provides the null solution when zero concentrations are prescribed at the boundaries. The two other columns are carryovers from $\underline{A}'$ when unit boundary concentrations are prescribed.

Equations (4.9) are solved by generalizing the well-known Thomas algorithm to handle 3 right-hand sides. After the boundary concentrations are computed, the interior mesh point concentrations are obtained by back-substitution in Equation (4.8)

4.4.2 Boundary Mesh Points

It may be recalled from section 3.1.1 that the weighted residual procedure applied to a simple linear element is analagous to proration of a distributed load to the supports of a simply supported beam. The basic notion in formulating the network solution procedure here is that a node is a common support to the beams or elements which enter it. Therefore, an overall reaction or conservation of mass equation can be written for each node by summing the contributions from each element adjacent to it. These are given by the first and last of Equations (4.7).

The boundary equations are written in terms of boundary concentrations only by substituting Equation (4.8) for $\bar{c}(2)$ and $\bar{c}(M-1)$. The results are:

$$\alpha_{11}\bar{c}(1) + \alpha_{1M}\bar{c}(M) = \eta_1\Delta t + \beta_1 \quad (4.10a)$$

$$\alpha_{M1}\bar{c}(1) + \alpha_{MM}\bar{c}(M) = \eta_M\Delta t + \beta_M \quad (4.10b)$$

$$\alpha_{11} = a(1) + c(1) \cdot dx_1(2)$$

$$\alpha_{1M} = c(1) \cdot dx_M(2)$$

$$\alpha_{M1} = b(M) \cdot dx_1(M-1)$$

$$\alpha_{MM} = a(M) + b(M) \cdot dx_M(M-1)$$

$$\beta_1 = B_1 - c(1) \cdot \bar{c}^0(2)$$

$$\beta_M = B_M - b(M) \cdot \bar{c}^0(M-1)$$

At each interior node, it is assumed that the boundary concentrations are compatible and that mass flux is conserved. At node 2 of the example network in Figure 4.1, the compatibility condition is:

$$\bar{c}^I(M) = \bar{c}^{II}(1) = \bar{c}^{III}(1) = \bar{c}_2 \quad (4.11)$$

where $\bar{c}_2$ is defined as the single concentration at node 2. Enforcing compatibility, conservation of mass flux is written as

$$(-Q_M^I + \overset{0}{Q_1^{II}} + Q_1^{III}) \bar{c}_2 + (\eta_M^I + \eta_1^{II} + \eta_1^{III}) \Delta t = 0 \quad (4.12)$$

In Equation (4.12), conservation of water imposes conservation of advective flux, and all the flux terms are defined as being into the boundary elements.

Looping over all the nodes will result in the following set of equations for the boundary concentrations:

$$\begin{bmatrix}
 \alpha_{11}^I & & & & \\
 & \alpha_{1M}^I & & & \\
 \alpha_{M1}^I & (\alpha_{MM}^I + \alpha_{11}^{II} + \alpha_{11}^{III}) & (\alpha_{1M}^{II} + \alpha_{1M}^{III}) & & \\
 & (\alpha_{M1}^{II} + \alpha_{M1}^{III}) & (\alpha_{MM}^{II} + \alpha_{MM}^{III} + \alpha_{11}^{IV}) & \alpha_{1M}^{IV} & \\
 & & & \alpha_{M1}^{IV} & \alpha_{MM}^{IV}
 \end{bmatrix}
 \begin{bmatrix}
 \bar{c}_1 \\
 \bar{c}_2 \\
 \bar{c}_3 \\
 \bar{c}_4
 \end{bmatrix}
 =
 \begin{bmatrix}
 \eta_1^I \Delta t + \beta_1^I \\
 \beta_M^I + \beta_1^{II} + \beta_1^{III} \\
 \beta_M^{II} + \beta_M^{III} + \beta_1^{IV} \\
 \eta_M^{IV} \Delta t + \beta_M^{IV}
 \end{bmatrix}$$

(4.13)

The dispersive flux terms at interior nodes 2 and 4 cancel by virtue of Equation (4.12).

Equation (4.13) can be solved once the boundary conditions are specified at nodes 1 and 4. The boundary conditions are imposed in a manner similar to that discussed in section 3.1.2. Dispersive flux can be specified at node 1 by evaluating the term on the right-hand side of the first equation. Concentration can be specified at node 4 by using a row-column elimination procedure. Total flux is handled by taking this boundary condition into account when formulating the boundary equation. Instead of a dispersive flux term on the right-hand side of Equation (4.13), there will be a total flux term which can be evaluated directly.

As in the hydraulics, the coefficient matrix of Equation (4.13) is banded, allowing efficient computational procedures. Experience has shown that the coefficient matrix is strongly diagonally dominant.

Therefore, the set of equations should be reasonably well conditioned, which should assure accurate numerical answers.

CHAPTER V

CASE STUDIES

5.1 Hydraulic Model of the James River at the U.S. Army Corps of Engineers Waterways Experiment Station

The advective and dispersive characteristics of a mathematical water quality model may be tested by simulating the distribution of a conservative substance such as salinity or dye (if conservative). These are ideal tracer substances since they eliminate the need to estimate reaction coefficients or decay rates. Dye tests which have been performed in hydraulic models are convenient to simulate, as the tests are made under carefully controlled and sometimes simplified conditions which can be reproduced easily in the mathematical model. Also, the hydraulic model data is usually more accurate and more complete than data taken in the field.

To validate the network water quality model against a reliable set of dye test data, it was decided to simulate portions of a series of dye tests which were performed in the James River Model at the U. S. Army Corps of Engineers Waterways Experiment Station. The tests were done in 1968 under the sponsorship of the Federal Water Quality Administration, and the results are unpublished at this time. Data for the tests were made available through the Middle Atlantic Region of the Federal Water Quality Administration, Charlottesville, Virginia.

A location map of the James River is shown in Figure 5.1. Its length is approximately 100 miles from the mouth at Old Point Comfort to the head of tide at Richmond. Between Richmond and Hopewell, the

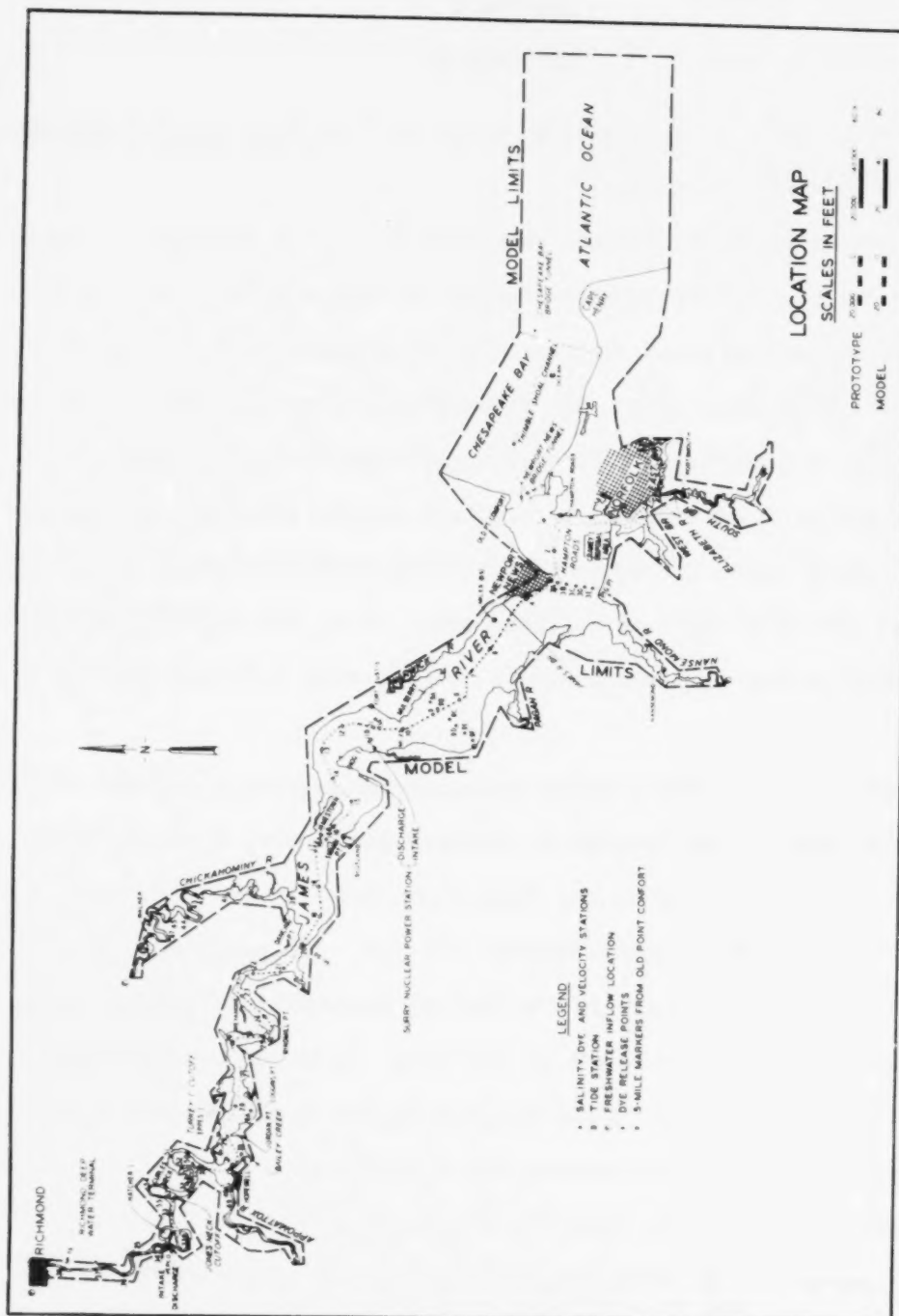


Figure 5.1 Location Map of the James River
(Adapted from WES data presentation)

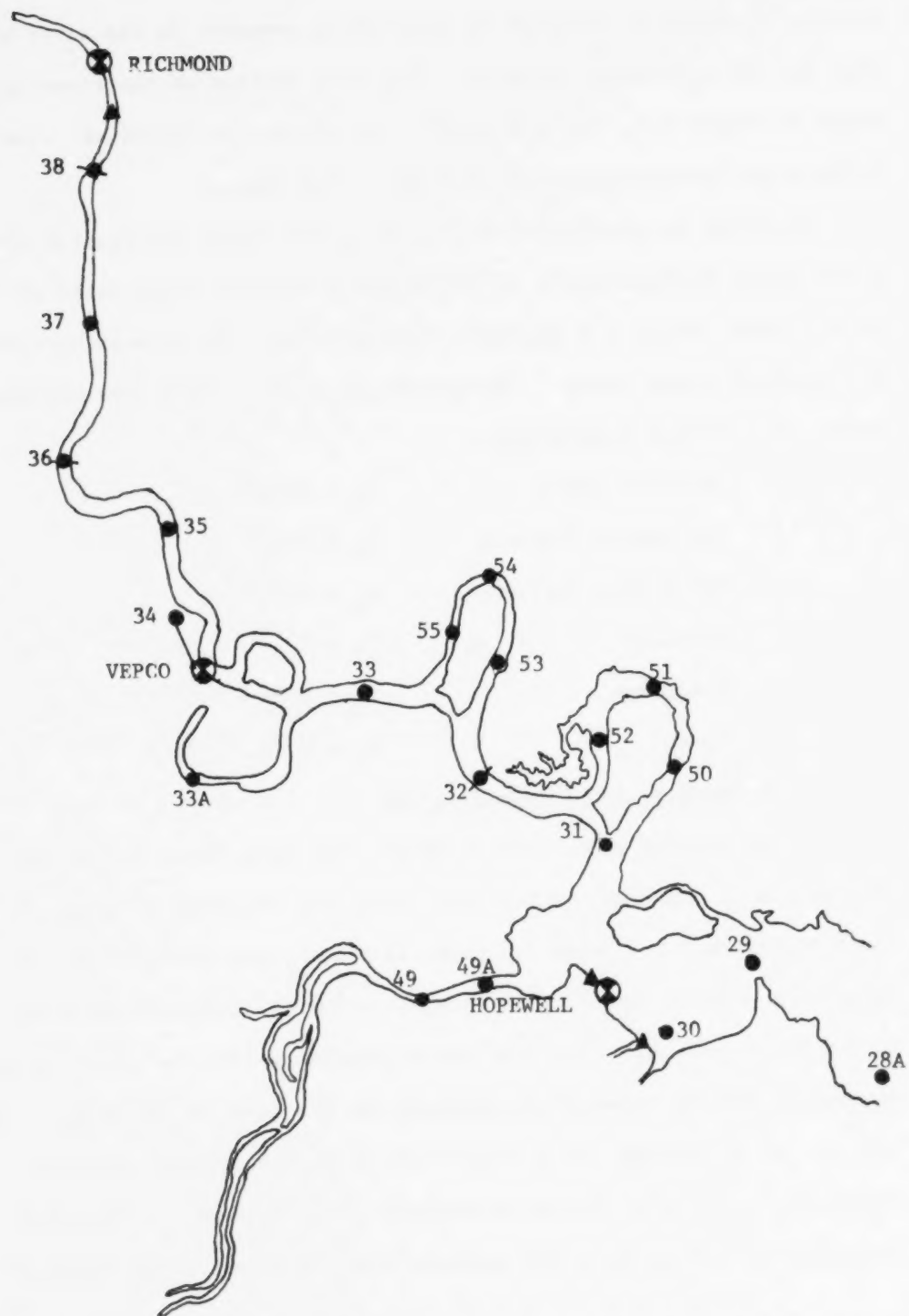


Figure 5.2 Loop Section of the James River between Richmond and Hopewell
-157-

estuary is marked by a series of loops where meanders in the river have been cut off by dredged channels. This loop section of the river is shown in Figure 5.2. Below Hopewell, the estuary is tree-like, with tributaries intersecting the main stem of the James.

The model is constructed according to the Froude scaling law with a horizontal distance scale of 1/1000 and a vertical depth scale of 1/100. Thus, there is a geometric distortion of 1/10 between horizontal and vertical length scales. The following scales relate commonly used model and prototype quantities.

Vertical depth	$Y_r = 1/10^2$
Horizontal distance	$L_r = 1/10^3$
Cross-sectional area	$A_r = 1/10^5$
Velocity	$V_r = Y_r^{1/2} = 1/10$
Discharge	$Q_r = A_r V_r = 1/10^6$
Time	$T_r = L_r / V_r = 1/10^2$

5.1.1 Geometry and Schematizations

For the network water quality model, the James River is represented as a series of channels, or reaches, which are connected to nodes, as shown in Figure 5.3. Table 5.2 summarizes the reach-node connectivities along with other schematization parameters for the hydraulic computations. It should be emphasized that the schematization parameters are in model dimensions and that simulation computations are done for the model itself. This avoids any assumption of similitude of longitudinal dispersion processes in distorted hydraulic models. (See Harleman, Holley, and Huber (1966)). Results of the computations are presented in terms of

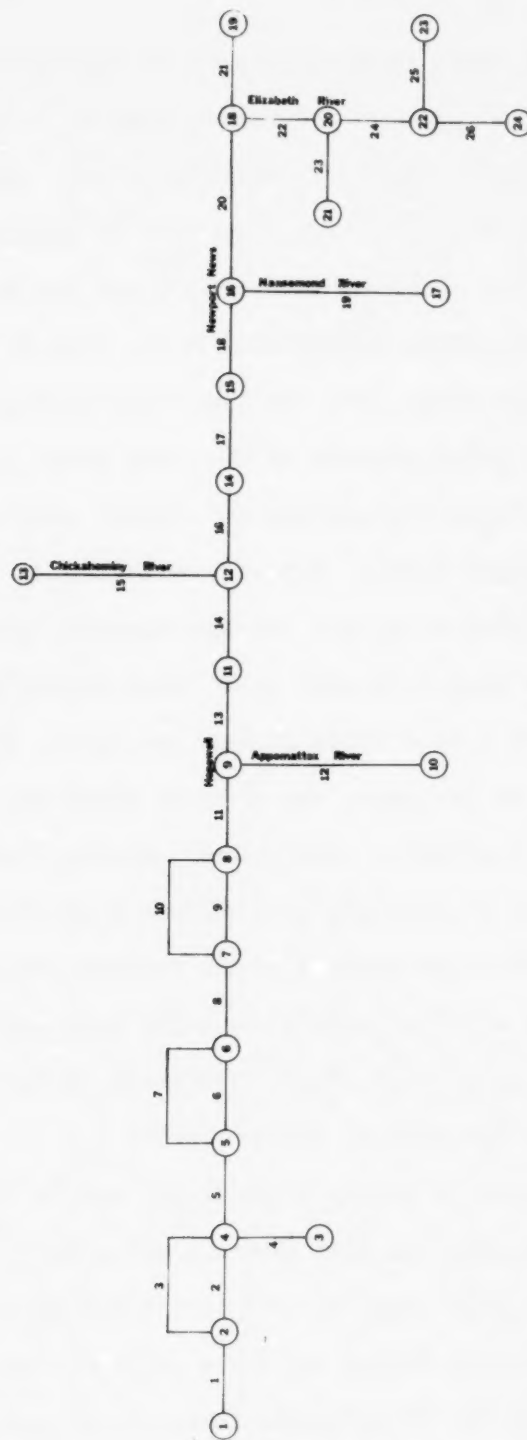


Figure 5.3 Reach-Node Representation of the James River

prototype units, which is the custom of the Waterways Experiment Station.

The technique for input of channel geometry information to the network water quality model is identical to that described by Wood, Harley, and Perkins (1972). Raw input data is supplied only at those data cross-sections necessary to provide a desired degree of resolution of channel cross-section variations. In the case of a prismatic channel at constant bottom slope, only one data cross-section is required. For the irregular, natural channels of the James River, geometric data for each reach was prepared by picking off channel cross-sections at selected locations from Coast Charts. Depths were divided by 100 and distances were divided by 1000 to convert the data directly to model dimensions.

One problem associated with using Coast Charts is that soundings are referenced to a local datum of mean low water. Over the length of an estuary such as the James, the absolute elevation of local mean low water will vary (and hence, chart datum), meaning that channel cross-section data must be corrected to a uniform water surface elevation. Conversations with staff members of the Waterways Experiment Station who are familiar with the James River Model indicated that this problem is not too important in the James. Therefore, datum for all charts was taken to be mean low water at Hampton Roads.

The James River is highly channelized, and the network configuration in Figure 5.3 includes all main channels and primary tributaries. Therefore, no storage areas were included in the hydraulic computations, and the core area of each channel was taken to be its total cross-sectional area. The results of the hydraulic computations under these assumptions

were quite reasonable and further refinement of the schematizations was omitted.

5.1.2 Verification of the Tidal Hydraulics

The 1968 dye tests covered three cases where fresh water inflows were held constant and one case where inflow at Richmond was varied to simulate the hydrograph recorded during a prototype dye test in 1966. For each case, a steady-state ocean tide was imposed with a prototype range of 2.5 feet and a semi-diurnal period of 12 hours 25 minutes in the prototype.

Verification of the tidal hydraulics is based on tide gage data recorded in the model for the three constant fresh water inflow cases. With inflows constant and a steady-state ocean tide, the stages and discharges repeat themselves every tidal cycle. The fresh water inflows into the James at Richmond and the primary tributaries are summarized in Table 5.1.

Table 5.1 Constant Fresh Water Inflows for the James River
Model in Prototype Units

Inflow Point	Case 1	Case 2	Case 3
James at Richmond	11,500 cfs	3,200 cfs	1,000 cfs
Appomattox	1,770	495	152
Chickahominy	651	182	56
Nansemond	1,040	291	89

To apply the network water quality model, the hydraulic model was schematized using the parameters listed in Table 5.2. The fresh water inflows were assigned to the appropriate reaches, and an ocean tide was imposed at node 19, the ocean boundary node. The tide curve was assumed to be sinusoidal with a range which closely matched the measured range at the nearby Hampton Roads gage. After a few trial computations with the 1000 cfs case, the set of Manning coefficients listed in Table 5.2 gave the results shown in Figures 5.4b, 5.5b, 5.6b, and 5.7b.

In general, the wide channels of the James below the Chickahominy River are assigned a Manning coefficient of 0.020. Between the Chickahominy and Hopewell, the James becomes narrower, and the Manning coefficient is raised to 0.025. Between Hopewell and Richmond, and in the tributaries, the Manning coefficient is increased further to 0.028. An exception is the Chickahominy, which is unusually tortuous, where a higher value of 0.035 is assumed.

Due to limited time and funds, trial runs for hydraulic verification were executed only for the 1000 cfs case. The channel cross-sections and Manning coefficients resulting from this test were used to generate the tidal hydraulics for the 11,500 cfs case. Figures 5.4a, 5.5a, 5.6a, and 5.7a show that the agreement with measured tidal stages is reasonable; therefore, any further refinement of the channel schematizations was not pursued.

The choices of mesh spacings Δx in the reaches and the time step Δt were based primarily on the desire to minimize computation time and cost. Values of Δx in each reach were chosen to yield a fairly coarse mesh,

Table 5.2 James River Model Schemitization Parameters
in Model Units

Reach	Upstream Node	Downstream Node	Hydraulic Δx Case 3 (ft)	Hydraulic Δx Case 1 (ft)	Manning Coefficient
1	1	2	4.18	4.18	.028
2	2	4	1.73	1.73	.028
3	2	4	2.10	2.10	.028
4	4	3	2.52	2.52	.028
5	4	5	1.88	1.88	.028
6	5	6	1.57	1.57	.028
7	5	6	2.01	2.01	.028
8	6	7	2.14	2.14	.028
9	7	8	0.74	0.74	.028
10	7	8	2.32	2.32	.028
11	8	9	1.90	1.90	.028
12	9	10	3.05	2.00	.028
13	9	11	3.09	2.01	.025
14	11	12	4.17	2.50	.025
15	12	13	5.09	2.76	.035
16	12	14	5.19	3.08	.020
17	14	15	5.09	3.51	.020
18	15	16	4.63	4.63	.020
19	16	17	5.45	5.45	.025
20	16	18	5.51	5.51	.020
21	18	19	3.26	3.26	.020
22	18	20	5.10	5.10	.025
23	20	21	5.58	5.58	.028
24	20	22	2.80	2.80	.028
25	22	23	4.66	4.66	.028
26	22	24	5.15	5.15	.028

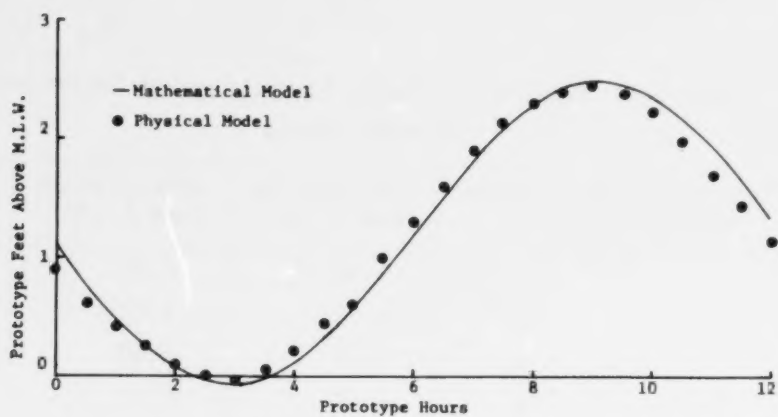


Figure 5.4a Tidal Stage at Hampton Roads Gage, 11500 cfs Test

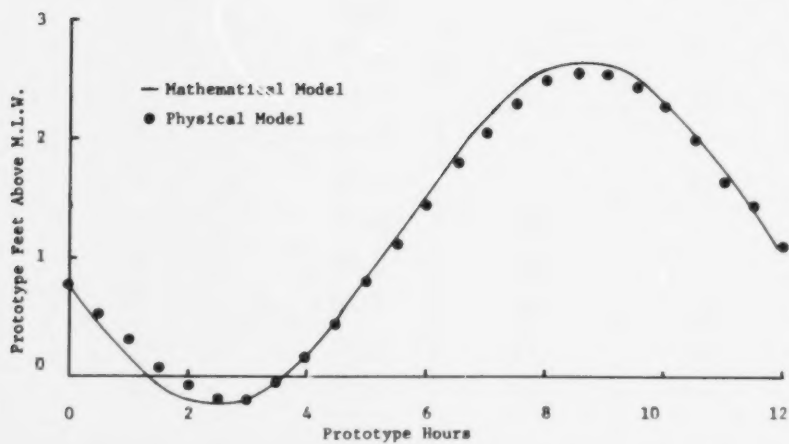


Figure 5.4b Tidal Stage at Hampton Roads Gage, 1000 cfs Test

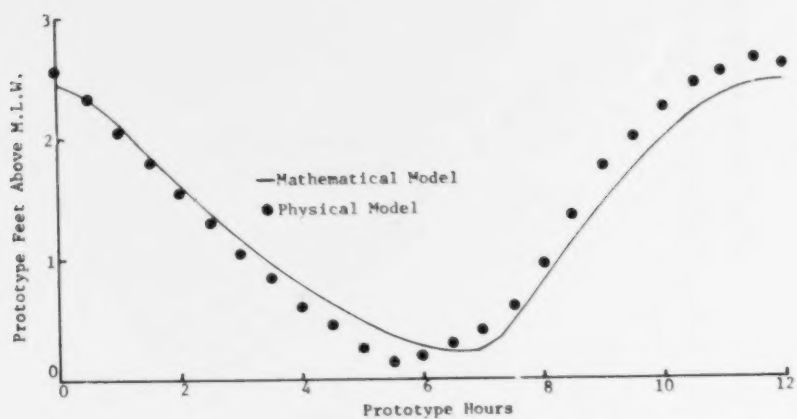


Figure 5.5a Tidal Stage at Scotland Gage, 11,500 cfs Test

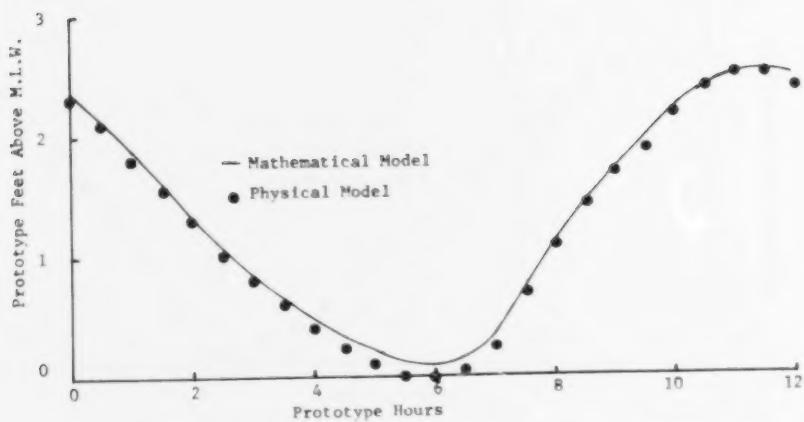


Figure 5.5b Tidal Stage at Scotland Gage, 1000 cfs Test

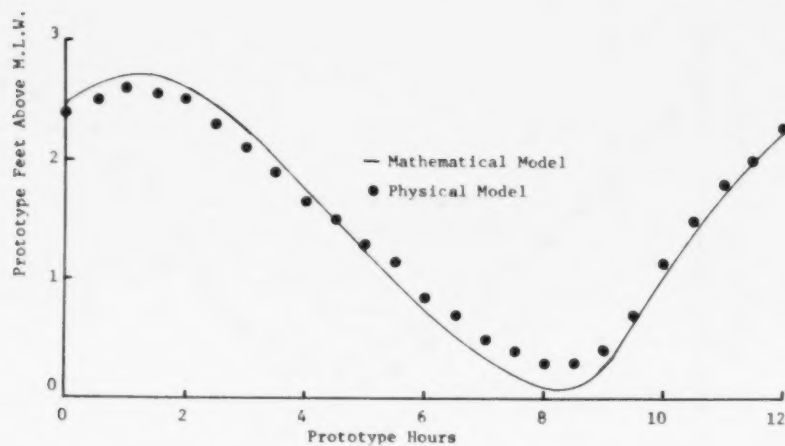


Figure 5.6a Tidal Stage at Weyanoke Gage, 11,500 cft Test

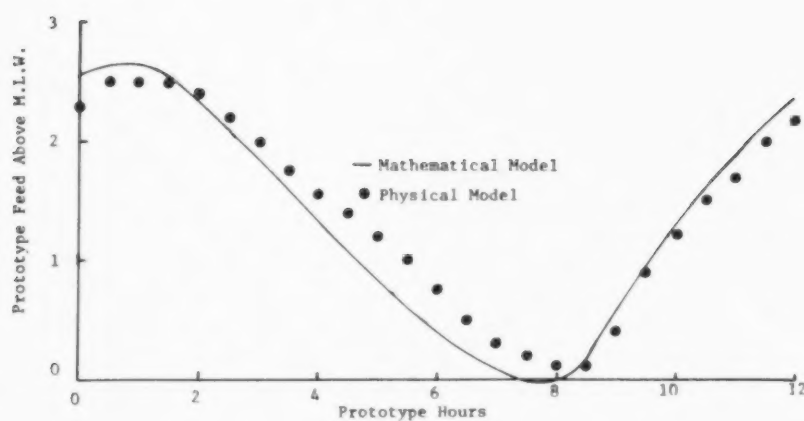


Figure 5.6b Tidal Stage at Weyanoke Gage, 1000 cfs Test

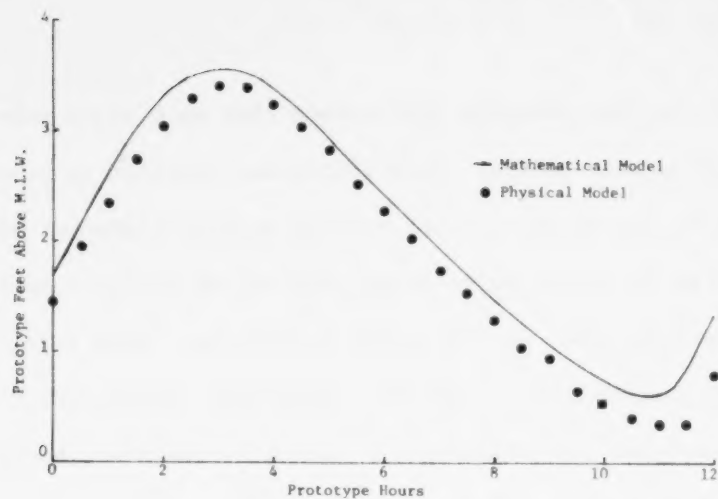


Figure 5.7a Tidal Stage at VEPCO Gage, 11,500 cfs Test

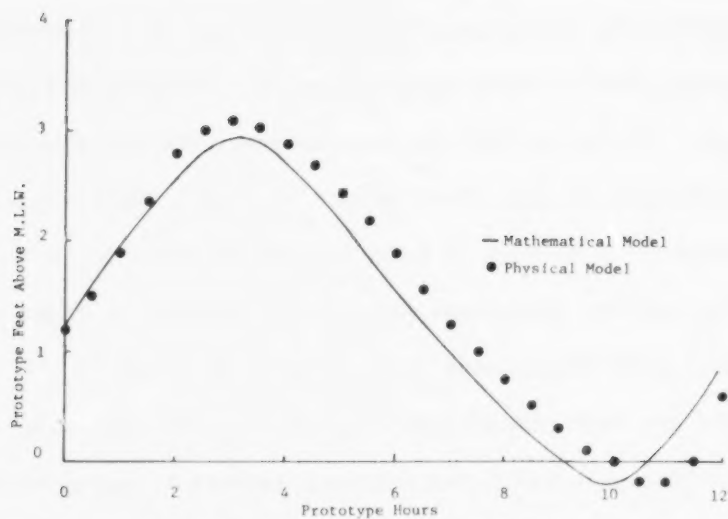


Figure 5.7b Tidal Stage at VEPCO Gage, 1000 cfs Test

subject to the arbitrary limitations that each reach must have at least 3 interior mesh points. This limitation resulted in unavoidably fine meshes in the short, cut-off reaches between Richmond and Hopewell. The time step Δt can be quite large, due to the implicit nature of the mathematical model for the tidal hydraulics. Therefore, an initial value of 4.47 seconds in the hydraulic model was chosen, which is equivalent to 100 time steps per tidal cycle. At this time step, however, it was found that the computations had difficulty in converging to the correct fresh water discharges, which are the average discharges over a tidal cycle. Decreasing the time step to 2.235 seconds, or 200 time steps per tidal cycle, seemed to alleviate the convergence problem between Richmond and Hopewell. However, the problem persisted below Hopewell where the hydraulic mesh became rather coarse. For the 1000 cfs case with dye injection at Richmond, the dye front is above Hopewell during most of the elapsed time for a reasonable simulation run. Therefore, the convergence problem below Hopewell was not considered too important for this case. In the 11,500 cfs case however, the dye front moves much further downstream in a given amount of time. Therefore, the values of Δx in reaches 12 through 17 were reduced as shown in Table 5.2. The resulting average discharges which were computed in these reaches agreed quite well with the correct fresh water discharges.

In the dye test simulations discussed in the following sections, the dye front does not reach the salinity intrusion region before the water quality computations are ended. Hence, the effects of salinity are not included in the hydraulic computations.

5.1.3 Dye Test Simulations

For each of the fresh water inflow cases, dye injections were made at both Richmond and Hopewell. In the three cases where fresh water inflow was constant, dye injection was continuous at the following rates and concentrations:

(1) At Richmond

rate = 2.5 gallons per hour

concentration = 100,000 parts per billion

(2) At Hopewell:

(a) At City Point

rate = 0.96 gallons per hour

concentration = 200,000 parts per billion

(b) At Baily Creek

rate = 0.54 gallons per hour

concentration = 1,000,000 parts per billion

Two different dyes, which could be traced separately, were used so that the tests could be conducted simultaneously. For all of the tests, the dye decay coefficients were taken to be zero. Further details of the test procedures are given by Lee and Harleman (1971).

In terms of testing the network water quality model, the most interesting part of the James River is the loop section between Richmond and Hopewell. Therefore, simulation effort in the present study was restricted to dye injections at Richmond. To save on computation costs, only the constant fresh water inflow cases were considered. For these cases, a single, steady-state tidal cycle for the hydraulics was computed,

stored on tape, and used repetitively in the course of the dye simulation runs.

The first dye test to be considered was Case 3 where fresh water inflow at Richmond was 1000 cfs. This is a low flow condition where the dye front moves slowly downstream, permitting careful observation of the transient increase of dye concentrations in the loops between Richmond and Hopewell. The injection point was located approximately 8.5 feet below the head of tide at Richmond in the model.

The computational mesh for the dye test simulations was set up using the techniques illustrated in section 3.1.6. Values of the maximum velocity and hydraulic radius near the injection point were estimated from the hydraulic computations

$$U \approx 0.027 \text{ ft/sec. (max. tidal velocity)}$$

$$R_h \approx 0.080 \text{ ft.}$$

The dispersion coefficient is taken conservatively as the Taylor value

$$E = E_T = 77 n |U| R_h^{5/6}$$

where n = Manning coefficient.

With a value of $n = 0.028$

$$E \approx 7 \times 10^{-3} \text{ ft}^2/\text{sec.}$$

Recalling from section 3.1.6 that the parameter $\frac{Ux}{E}$ is approximated with x at about one tidal excursion.

$$x = \frac{UT}{\Pi} = \frac{0.027 \times 447}{\Pi} \approx 4.0 \text{ ft.}$$

and

$$\frac{Ux}{E} \approx 15$$

From Figure 3.6

$$(5\% \text{ cutoff}) = 1.4$$

The mesh spacing Δx may be calculated with Equation (3.55a)

$$\Delta x \leq \frac{4E}{U(5\% \text{ cutoff})} \approx 0.75 \text{ ft.}$$

The time step is governed by Equation (3.55b)

$$\Delta t \leq \frac{\Delta x}{U} \approx 27 \text{ sec.}$$

The mesh spacing actually used was 0.5 feet, in order to provide a number of mesh points between the injection point and the upstream boundary of reach 1. Below the injection point, the mesh spacing was gradually increased to 2.0 feet near the downstream end of reach 1. In the reaches between Richmond and Hopewell, the mesh spacing was about 2.0 feet, in general. Below Hopewell, the mesh spacing was gradually increased to between 4 and 6 feet, and as much as 8 feet in channel areas where significant concentrations were not expected. The time step for the computations was taken as 17.88 seconds, or 25 time steps per tidal cycle, which is considered to be a minimum for reasonable results.

The results of the dye test simulation with 1000 cfs at Richmond are shown in Figures 5.8 through 5.11. Station 31 is located just above Hopewell, station 34 is adjacent to the VEPCO tide gage, and stations 51 and 54 are at the tops of the two loops above Hopewell. To avoid large computational costs, the simulation is stopped after 30 tidal cycles when the transient increase of concentration at the four stations is reasonably well-defined. The results show that dispersion has a marked effect on the rate of concentration increase. Computed high-water slack

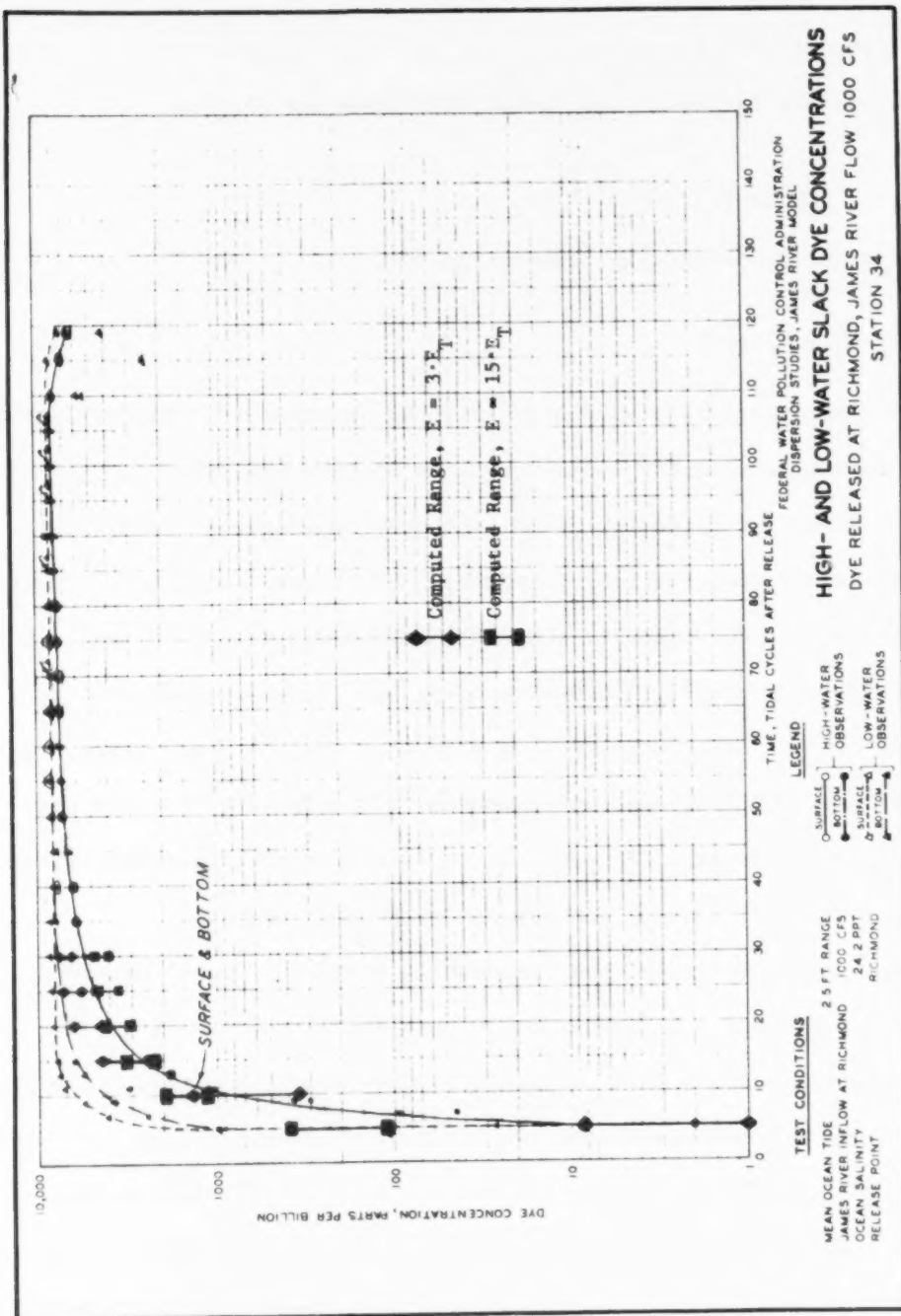


Figure 5.8 Concentration Increase near VEPCO, 1000 cfs Test
(adapted from WES data presentation)

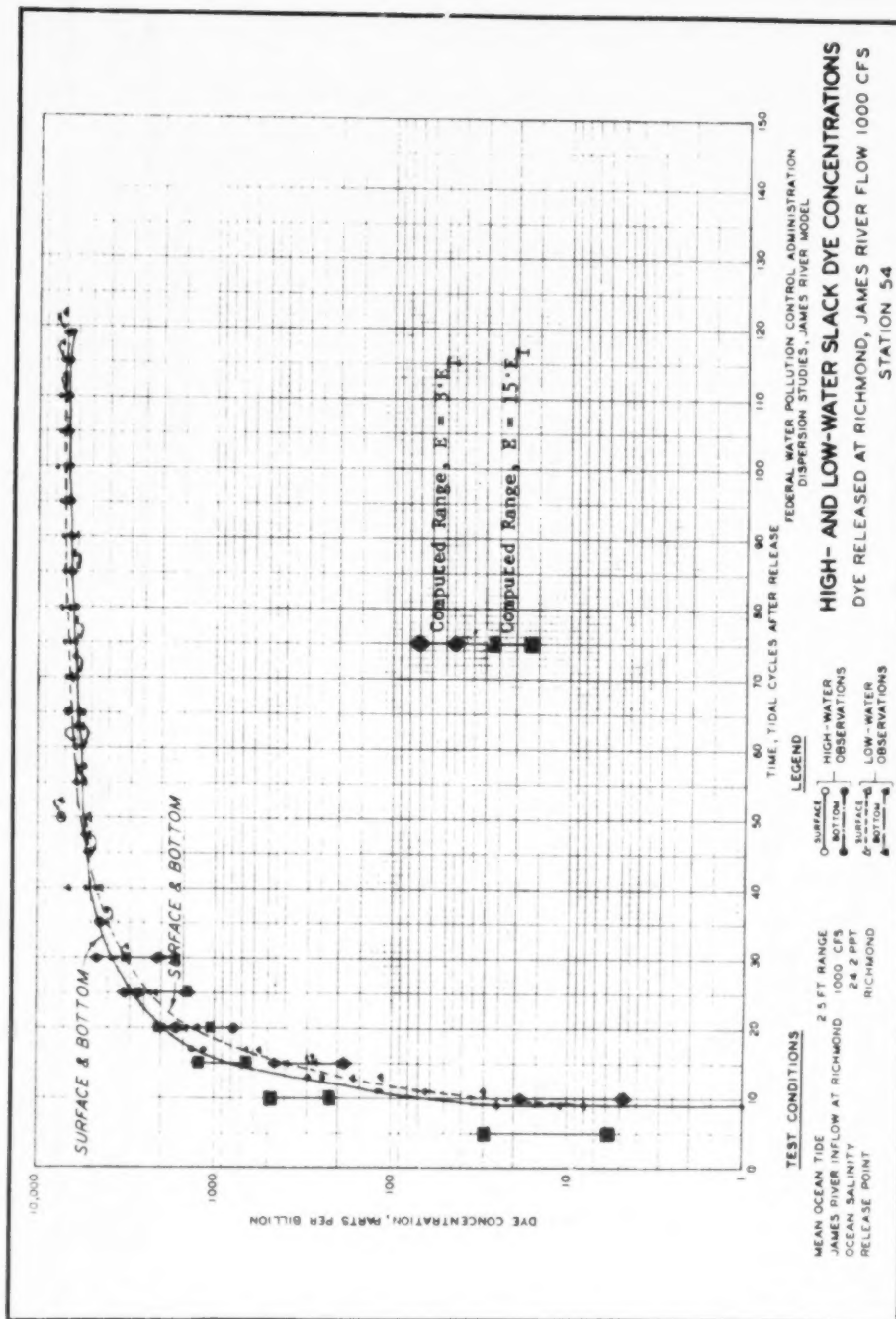


Figure 5.9 Concentration Increase in Curles Neck Loop, 1000 cfs Test
(adapted from WES data presentation)

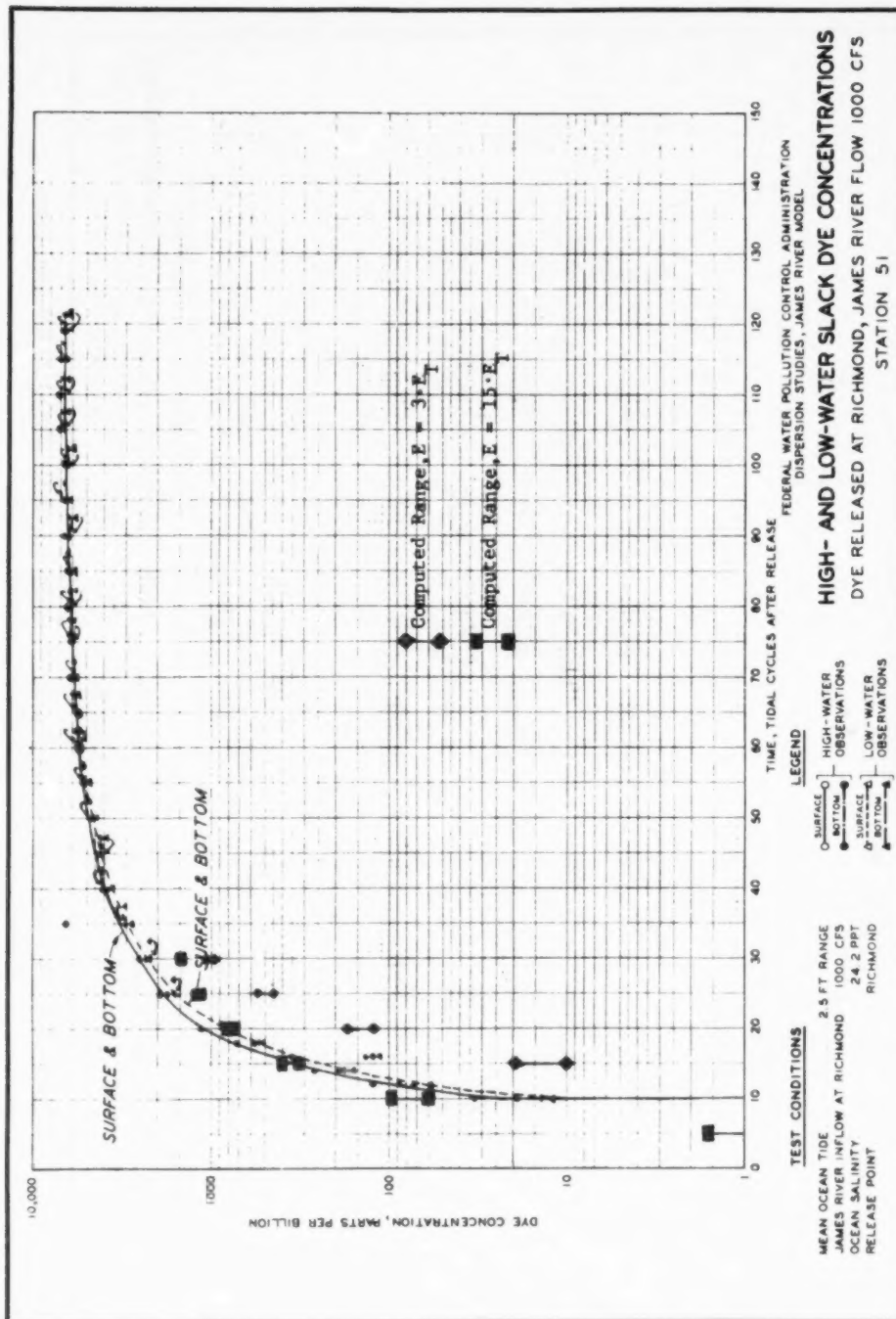


Figure 5.10 Concentration Increase in Turkey Island Loop, 1000 cfs Test
 (adapted from WES data presentation)

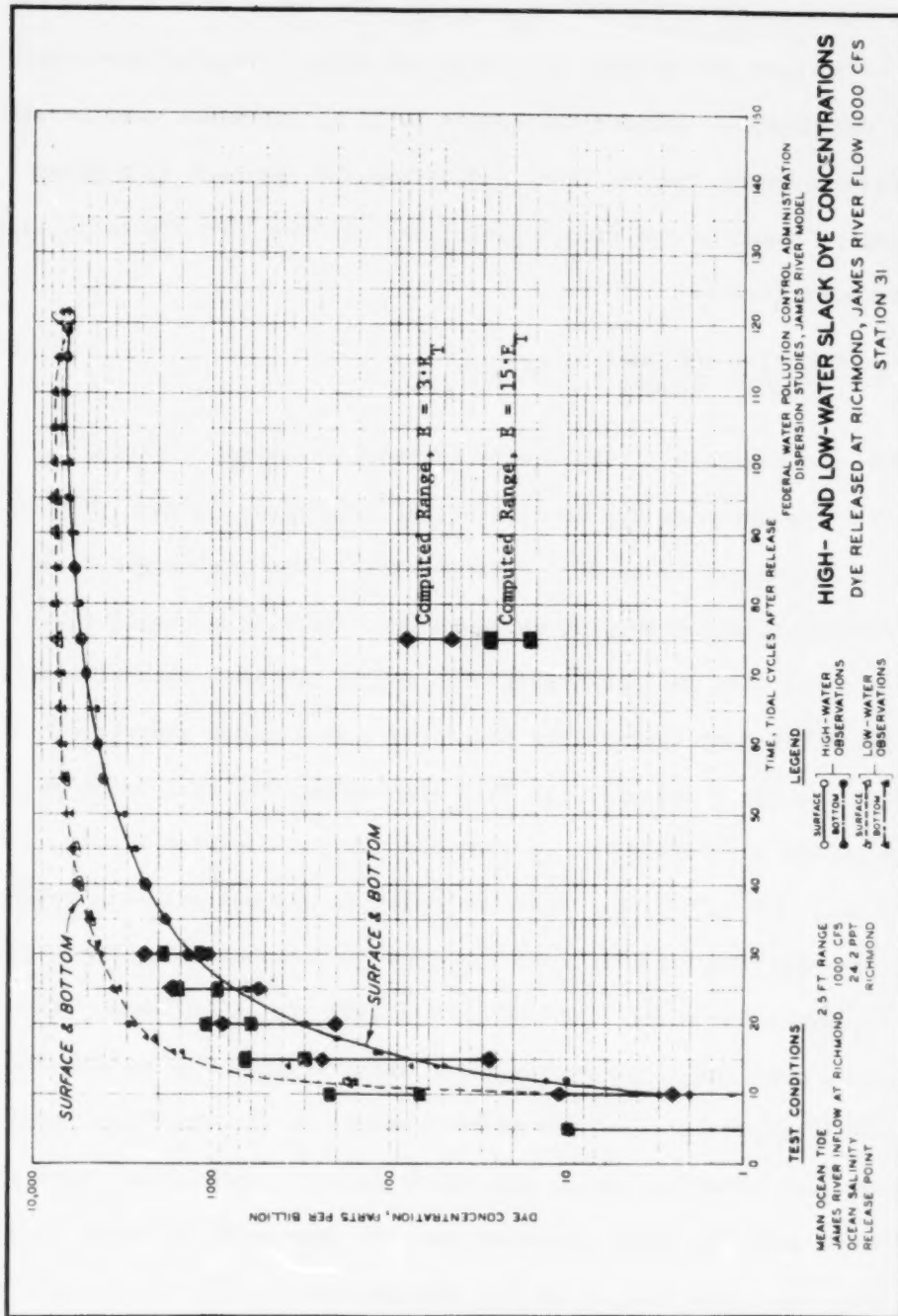


Figure 5.11 Concentration Increase near Hopewell, 1000 cfs Test
(adapted from WES data presentation)

values with $E = 3 \cdot E_T$ match measured values quite well; however, agreement with low-water slack values is not as good. The value of $3 \cdot E_T$ is often assumed to account for channel curvature and other irregularities which increase dispersion. Raising dispersion to $15 \cdot E_T$ increases concentrations in the forerunner of the dye front and delays the approach to a mixed concentration based on the fresh water flow. In the 1000 cfs test, this mixed concentration is

$$c_o = \frac{.000093 \times 100,000}{.001000 + .000093} = 8500 \text{ ppb}$$

which the concentration at Station 34 approaches asymptotically. At Station 51, the shape of the concentration curve seems correct, but it appears to be delayed by about 5 tidal cycles. This is thought to be due to a schematization problem in reach 10. There is a considerable amount of tidal flat and marsh area adjacent to the main channel and it is not clear how much these areas participate in surface storage of water and momentum transport. In this simulation, the full marsh area is included in the cross-section, so that discharge velocities may be unrealistically low. This may cause the delay in concentration increase.

To consider the behavior of a dye front in reaches below Hopewell, it was decided to simulate the test with 11,500 cfs at Richmond. This provides a second set of conditions with which to test the mathematical model, and computation times can be kept short, as the dye front moves downstream very quickly. Since the water quality computational mesh for the 1000 cfs test was quite conservative, the same mesh was used for the 11,500 cfs test. The results of the computations with $E = 3 \cdot E_T$ based on

the previous simulation are shown in Figures 5.12 through 5.18. Station 49A is in the Appomattox River at Hopewell, Station 23 is downstream of Weyanoke Point, and station 40 is located in the Chickahominy River. Once again, the simulation is terminated after 30 tidal cycles.

At several stations, the computed range of concentrations is less than the measured range. Part of the reason for this bias may lie in a discrepancy between the measured concentrations at station 34 and the mixed concentration based on fresh water flow. The measured concentrations exceed 1000 ppb, and the mixed concentration is

$$c_o = \frac{.000093 \times 100,000}{.011500 + .000093} = 800 \text{ ppb}$$

The computed range agrees quite well with the 800 ppb mixed concentration. It is possible that either fresh water flow in the hydraulic model was too low or the injection rate was too high. The latter may be more likely since time of travel compares favorably between the two results.

Schematizations of the loops were tested in this simulation by including only main channel areas and omitting marsh areas. In the Turkey Island Loop, the dye reaches station 51 too soon, indicating that the correct schematization is somewhere between the ones used in the two simulations.

The computed concentrations at station 49A demonstrate how the semi-logarithmic plot distorts small concentrations. At this station, the computed concentration went negative over a portion of every tidal cycle, indicating that the mesh spacing of about 3 feet could not resolve the steep concentration gradient in the Appomattox without oscillations.

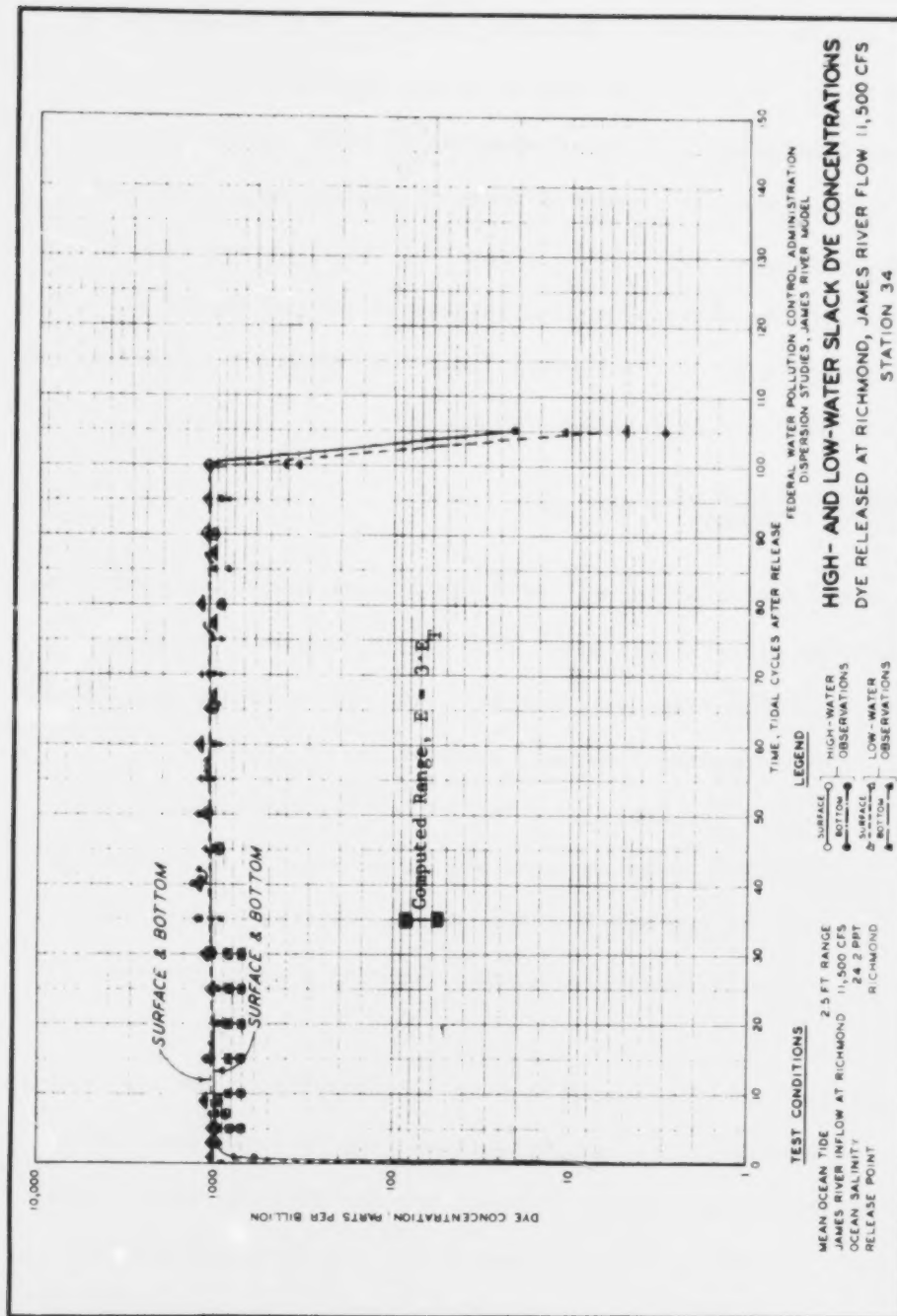


Figure 5.12 Concentration Increase near VEPCO, 11,500 cfs Test
(adapted from WES data presentation)

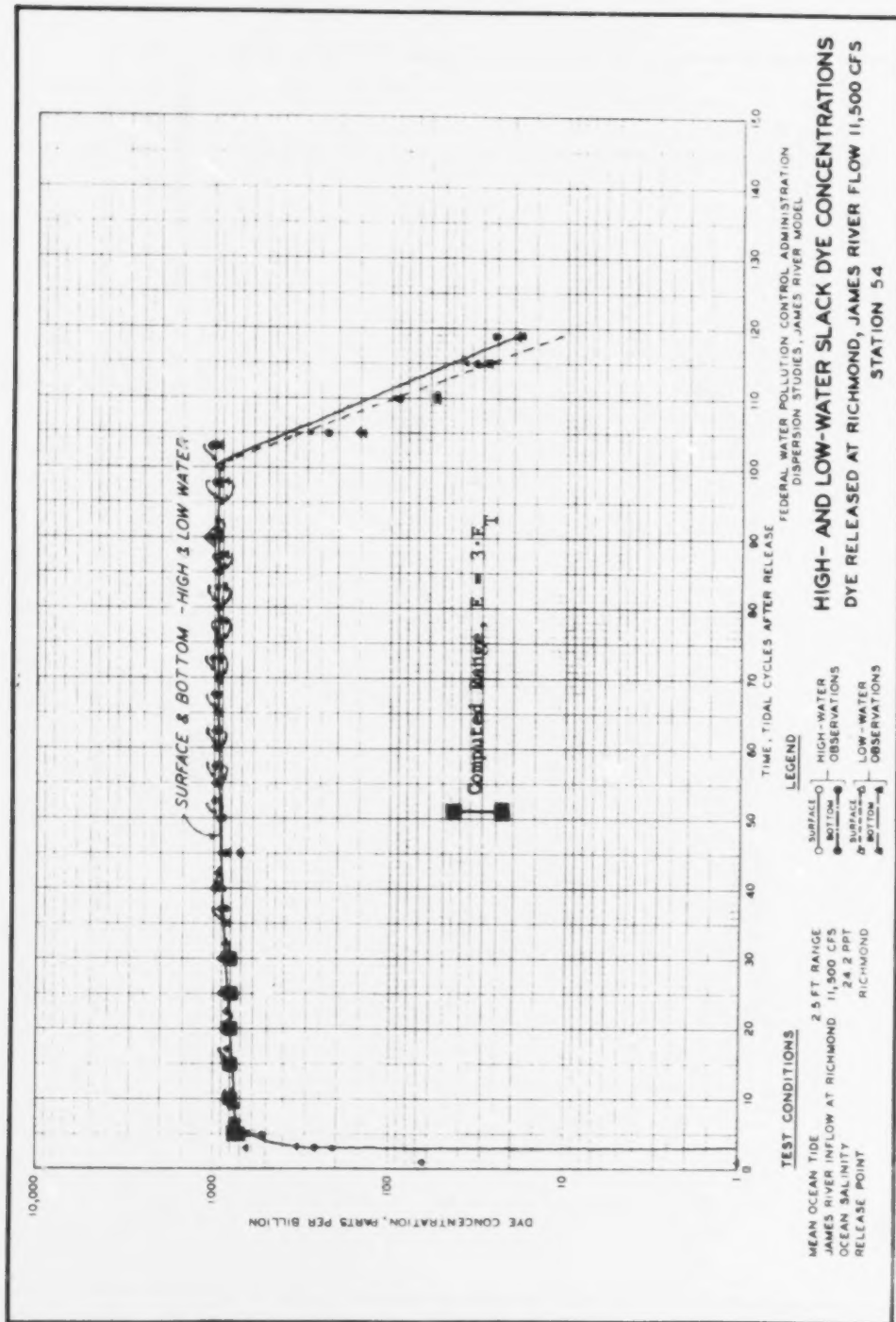


Figure 5.13 Concentration Increase in Curles Neck Loop, 11,500 cfs Test
(adapted from WES data presentation)

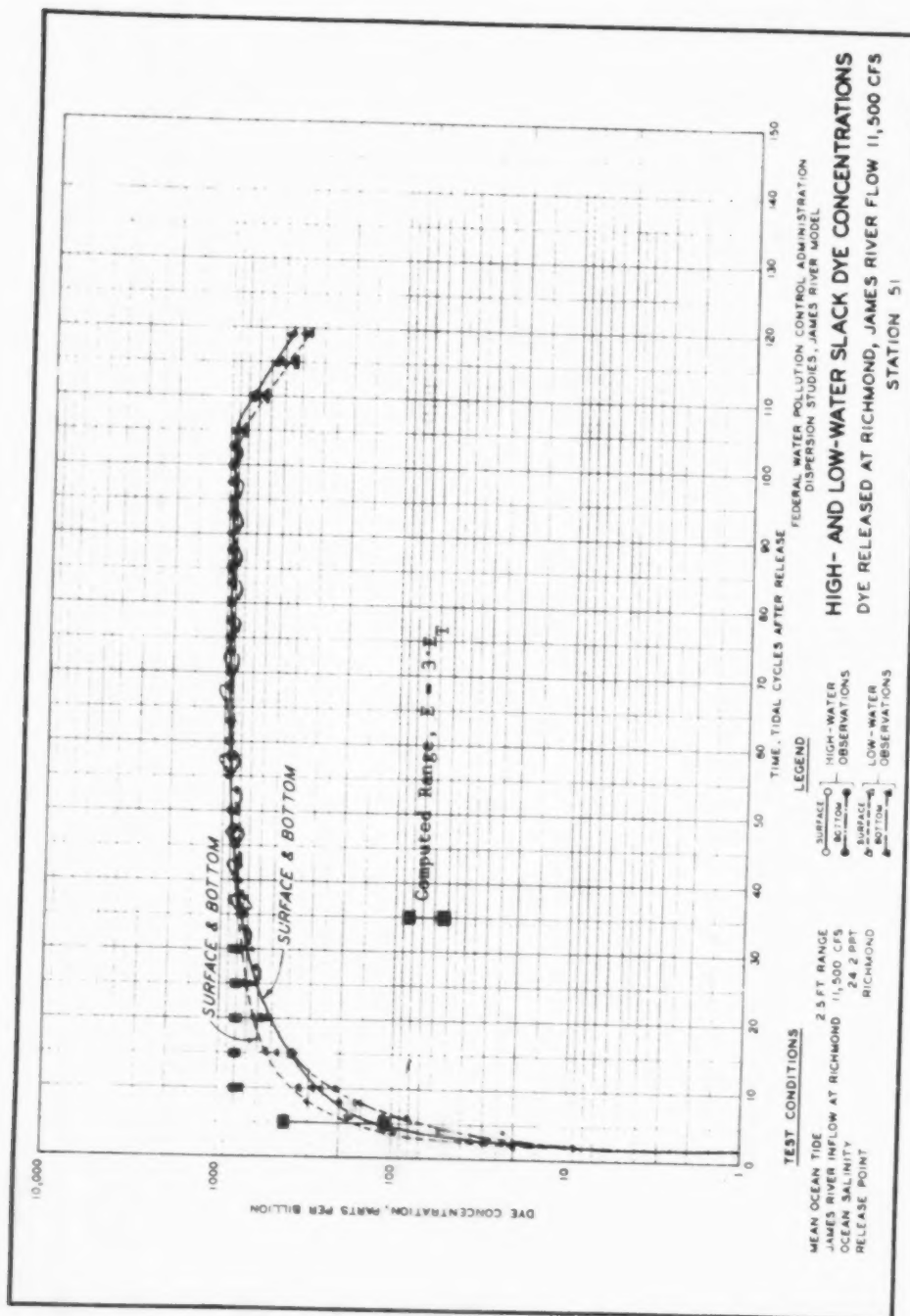


Figure 5.14 Concentration Increase in Turkey Island Loop, 11,500 cfs Test
(adapted from WES data presentation)

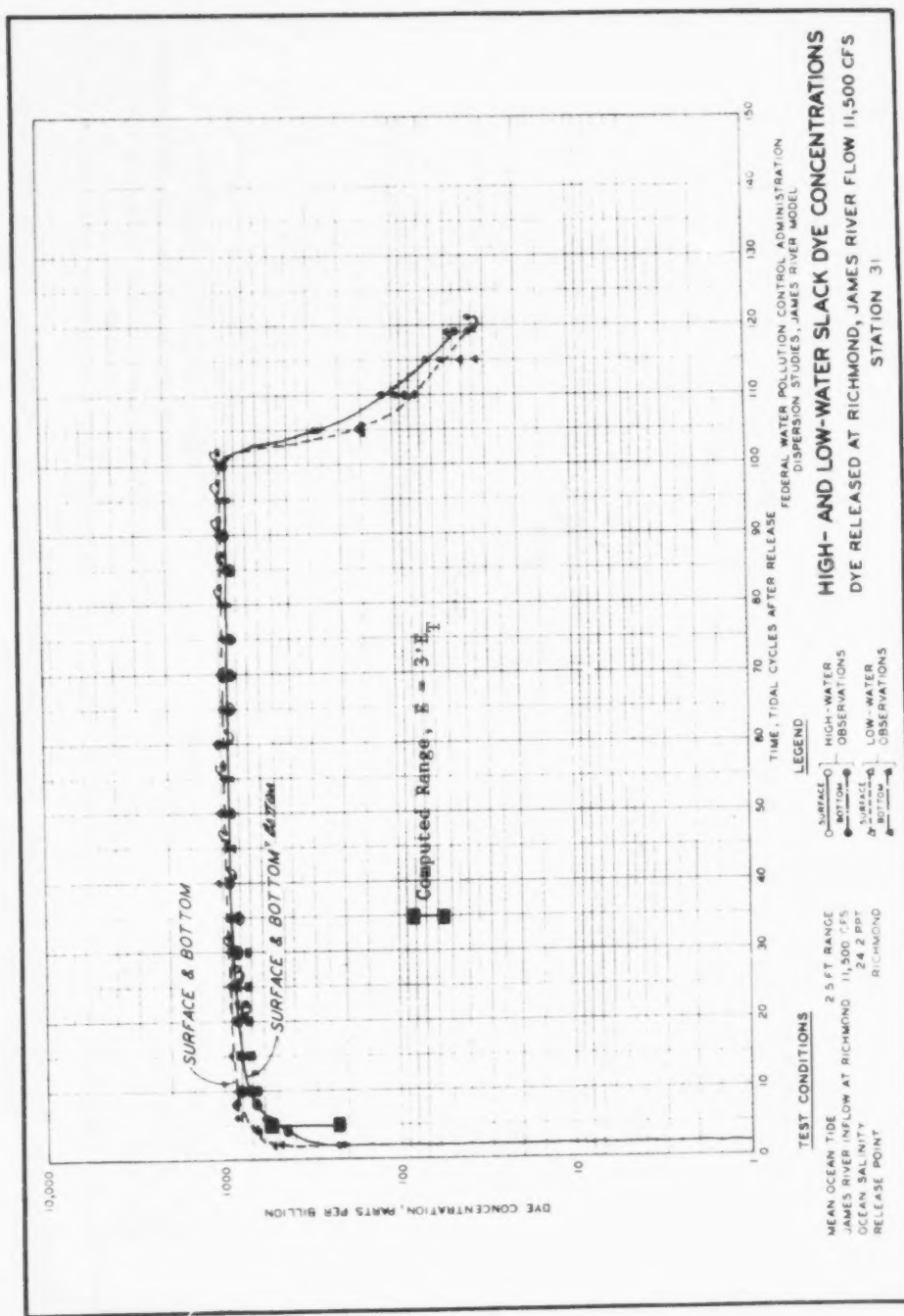


Figure 5.15 Concentration Increase near Hopewell, 11,500 cfs Test
(adapted from WES data presentation)

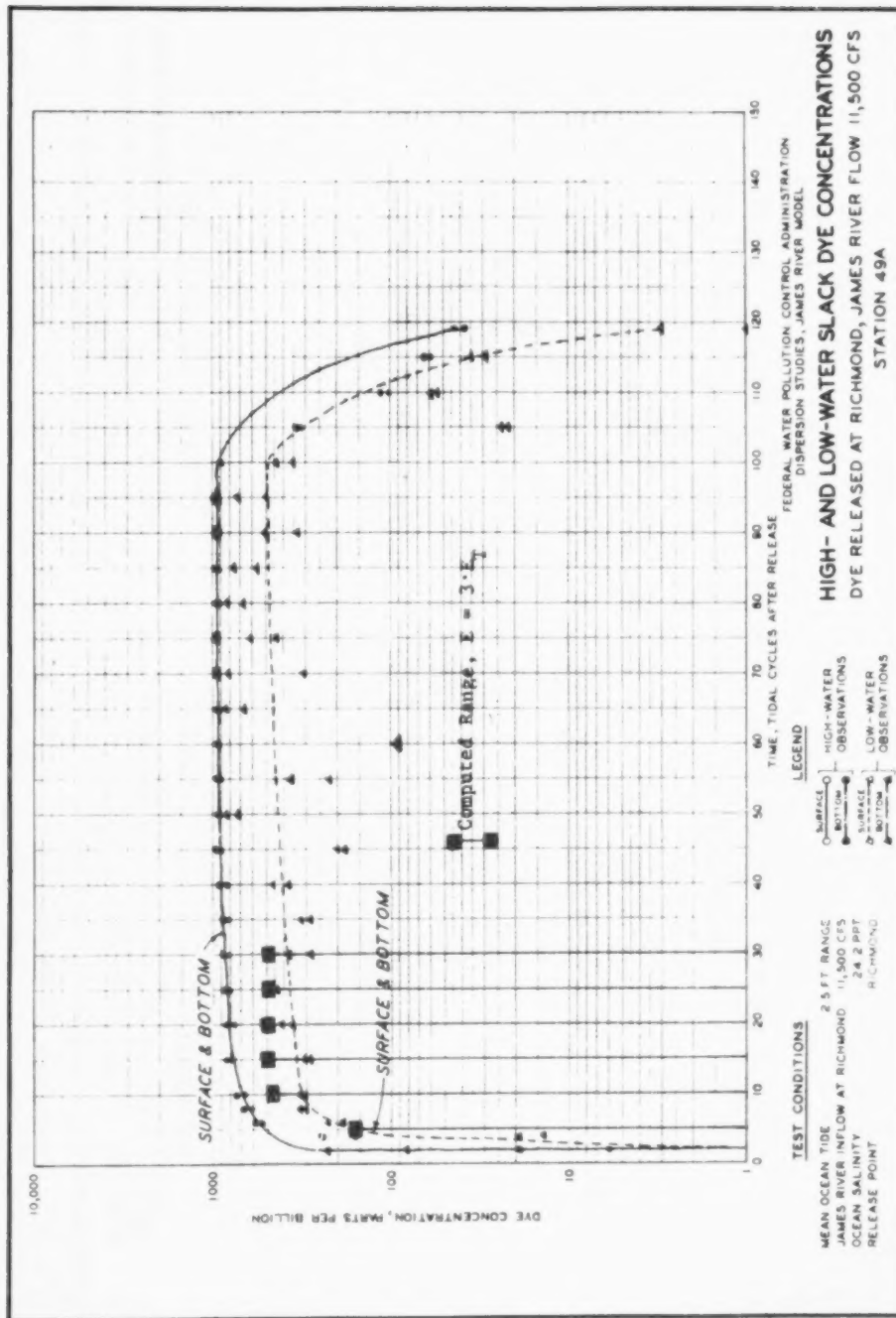


Figure 5.16 Concentration Increase in the Appomattox River at Hopewell, 11,500 cfs Test
(adapted from WES data presentation)

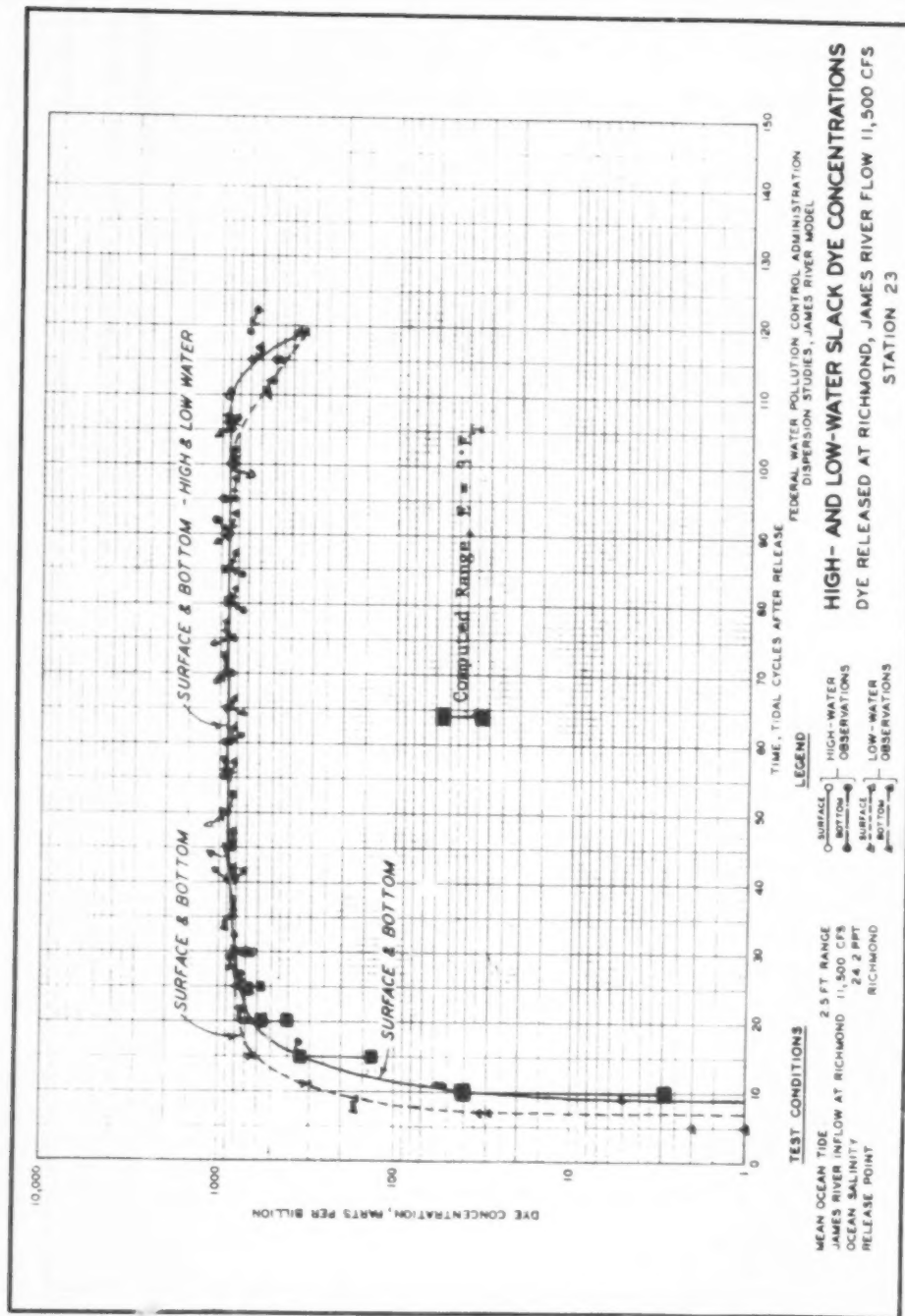


Figure 5.17 Concentration Increase near Weyanoke Point, 11,500 cfs Test
 (adapted from WES data presentation)

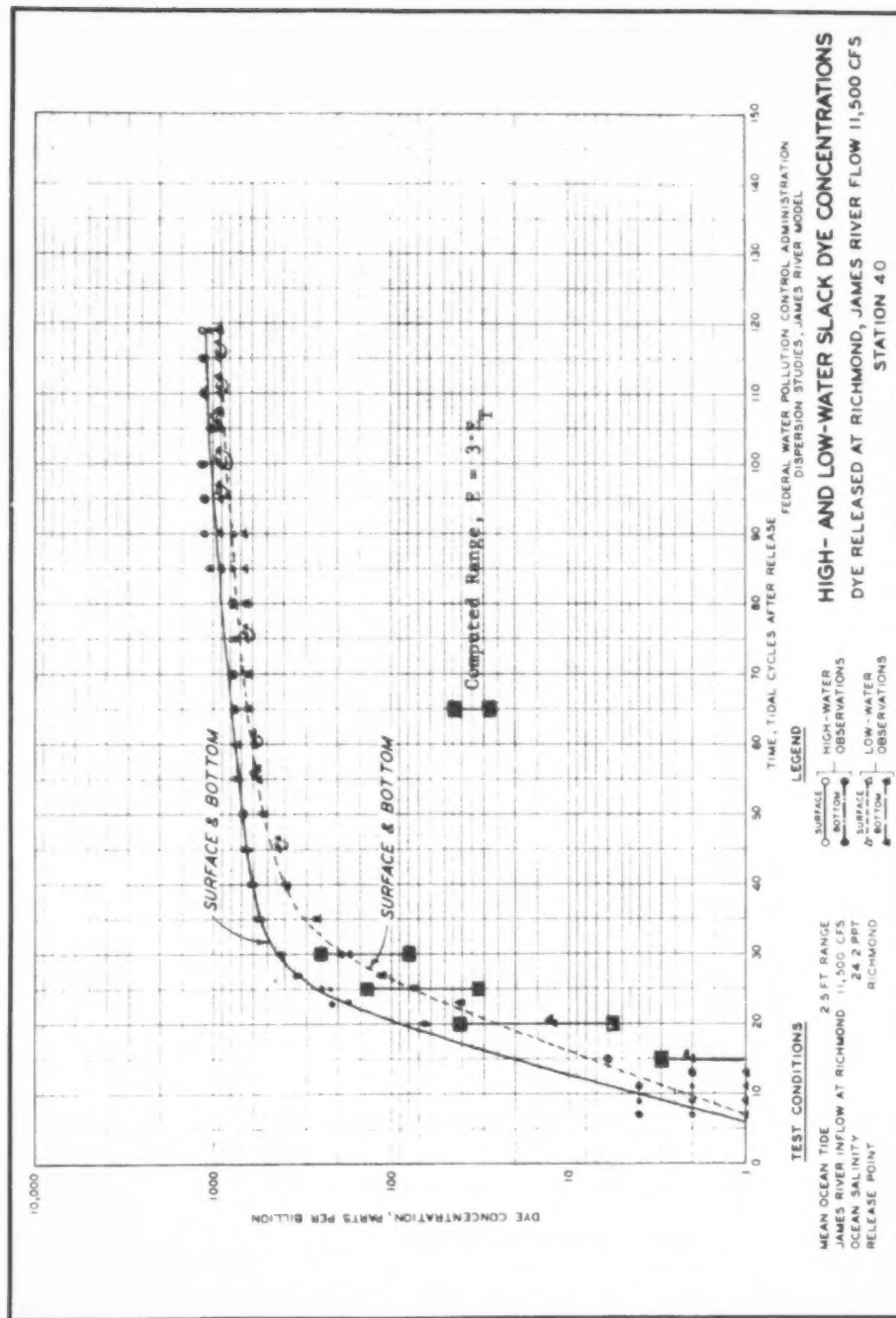


Figure 5.18 Concentration Increase in the Chickahominy River, 11,500 cfs Test
(adapted from WES data presentation)

Also, a slight discrepancy in horizontal position with a steep concentration gradient can produce a sizeable difference in concentrations. This is a definite consideration at station 40, where the mesh point at which computed concentrations were taken was located about 1.5 feet above the station location in the hydraulic model. Thus, the observed effect is computed concentrations which appear too low. Finally, the results at station 23 are quite good, especially if the measured concentrations are too high, as discussed above.

5.2 Cork Harbour, Ireland

As discussed in section 2.3.1, Cork Harbour presents a number of features which motivated development of the network water quality model. The geometry is very complex, consisting of embayment areas connected by narrow straits. Within the present state-of-the-art, a one-dimensional network model is probably the best way to consider water quality problems in the harbor. Also, fresh water inflows are very small, averaging 1000 to 2000 cfs, with the River Lee providing most of the inflow at Cork. Therefore, the principal mechanism for removing wastes from the harbor is tidal flushing. With very small net advective flows to remove wastes, maintenance of water quality in the harbor is a matter of growing concern as the area becomes more industrialized.

The following three sections present a simulation of one dye test which was part of a series conducted in the harbor by Metcalf and Eddy, Inc. to evaluate alternative discharge locations for industrial waste disposal. Injection for the dye test chosen was located at an outfall

site which became operational later, discharging relatively low levels of waste at varying rates. The intent was to confirm the mathematical model's ability to reproduce the transport processes of advection and dispersion by simulating the distribution of dye, which is presumed conservative. As a reliable body of data on water quality parameters such as BOD and DO becomes available from a field monitoring program, the mathematical model can be used to predict both the transport processes and the reaction processes.

A preliminary, simplified mathematical model of Cork Harbour indicated that the outfall site discussed above would be inadequate for eventual waste loads which were planned. With small fresh water through-flow, significant levels of BOD and DO deficit concentrations accumulated within a tidal excursion of the injection point. Therefore, it was decided to utilize the benefits of tidal flushing by locating the discharge site nearer the harbor entrance. Section 5.2.4 discusses mathematical simulation of BOD and DO distribution resulting from waste discharges at this site and shows how an intermittent injection scheme can be investigated with the network model. An important variable affecting the removal of wastes by tidal flushing is the per cent return at the ocean boundary. Field studies are being conducted at present to obtain an estimate of per cent return for Cork Harbour for inclusion in later studies.

5.2.1 Geometry and Schematizations

Cork Harbour is a fairly short estuary with the main channel running some 18 miles between the ocean entrance and the head of tide at the Cork

Waterworks weir. It was schematized as shown in Figures 2.6 and 5.21 with 13 reaches and 12 nodes. The connectivities of the reaches are given in Table 5.3. It may be noted that some effort was made to number the nodes in such a way as to keep the difference between two numbers in any given reach as small as possible. This minimizes the bandwidth of the network coefficient matrix discussed in section 4.3.2 and economizes on computer time.

The schematization is rather crude, especially in upstream areas such as Lough Mahon. Since the present study is concerned with water quality in the Lower Harbour around Haulbowline and Spike Islands, the primary concern was to reproduce the tidal prism in upstream areas, so that discharges in the Lower Harbour would be simulated correctly. The embayment area of the Lower Harbour is schematized with only a few reaches which follow well-defined channels on the coast charts. A highly refined network representation which attempts to model two-dimensional flow patterns may yield results of questionable accuracy, since a one-dimensional network model does not include the effects of wind shear and Coriolis accelerations.

5.2.2 Verification of the Tidal Hydraulics

There is very little published information on the tidal hydraulics of the entire estuary. Tidal stage predictions are given by the Tide Tables for two locations, Cork and Cobh. The spring ranges are given as 11.9 feet and 12.9 feet, respectively, and the lag between the two is about 20 minutes for both high water and low water. Data given for nearby locations on the open coast, both in the Tide Tables and in a local newspaper, The Cork Examiner, indicate that the ocean tide is about the

same as the Cobh tide. Under spring tide conditions, O'Kane (1968) notes that the peak discharge at Passage West is about 100,000 cfs and the peak discharge at the ocean entrance is about 400,000 cfs.

To verify the tidal hydraulics, a semi-diurnal ocean tide with a range of 12 feet was imposed at node 1 of the mathematical model. The reaches in the network were discretized as shown in Table 5.3, and a Manning coefficient of $n = 0.025$ was chosen arbitrarily for each reach.

Table 5.3 Cork Harbour Schematication Parameters

Reach	Upstream Node	Downstream Node	Hydraulic Δx (ft.)	Manning Coefficient
1	2	1	1400	0.025
2	3	2	1900	0.025
3	5	2	2200	0.025
4	4	2	1800	0.025
5	7	5	1900	0.025
6	4	5	700	0.025
7	6	5	1900	0.025
8	6	4	1400	0.025
9	8	6	1500	0.025
10	11	8	2000	0.025
11	12	8	2000	0.025
12	7	9	2000	0.025
13	7	10	2000	0.025

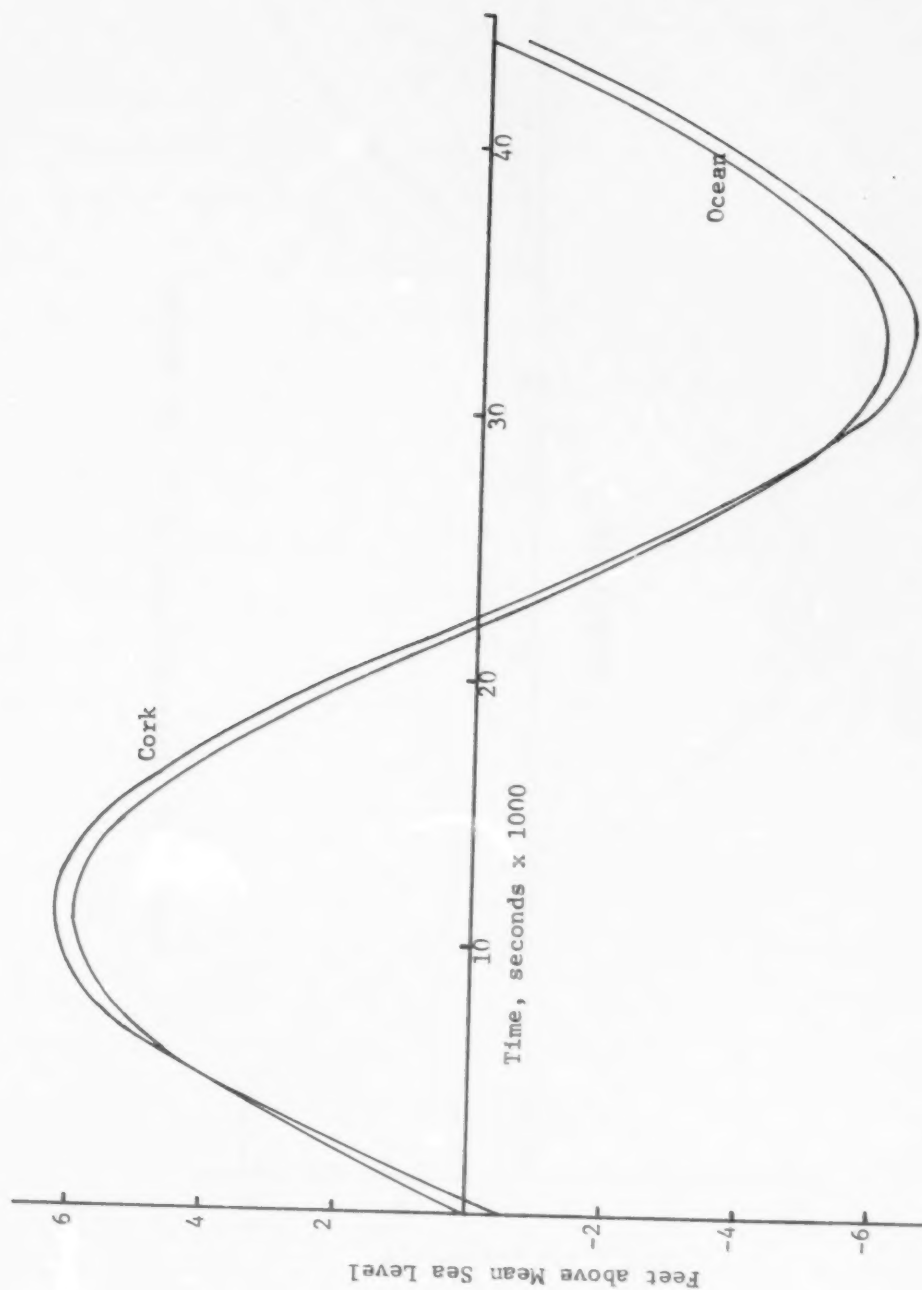


Figure 5.19 Computed Water Surface Elevations in Cork Harbour

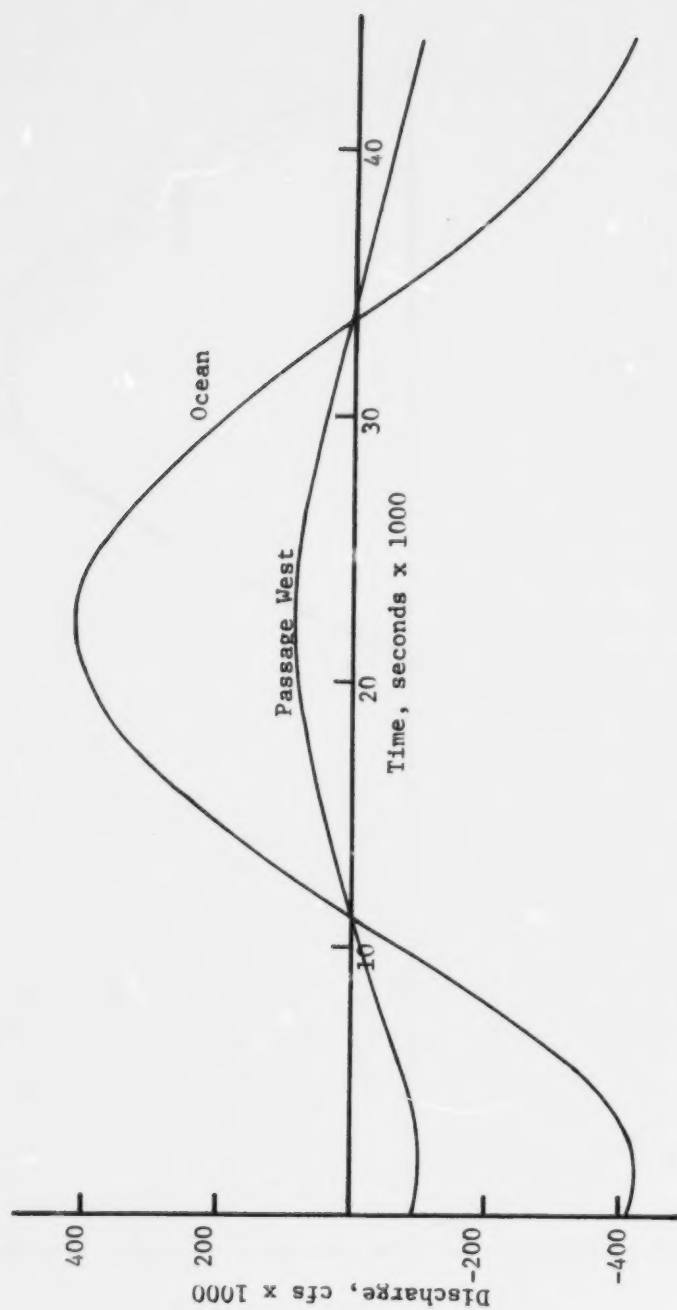


Figure 5.20 Computed Discharges in Cork Harbour

The hydraulic mesh spacings Δx were chosen to be as coarse as possible, while providing reasonable definition of irregularities in the channels. To minimize execution time, the time step was taken as 100 time steps per tidal cycle initially. However, it was found that oscillations in the discharge and water surface elevation profiles developed in the shallow channels near low water, indicating poor convergence of the numerical solution. Decreasing the time step to 150 time steps per tidal cycle eliminated most of the oscillations.

Computed results for water surface elevations and discharges are shown in Figures 5.19 and 5.20. The increase in range between the ocean and Cork is approximately 0.7 feet compared with an expected increase of about 1.0 feet from the Tide Tables data. The Cork tide also lags the ocean tide by approximately 15 minutes at low tide. For water quality computations, the most important results of the hydraulic computations are the discharges. The results shown in Figure 5.20 at the ocean entrance and at Passage West agree quite well with the values quoted by O'Kane.

5.2.3 Dye Test Simulation

For the dye test simulated, Rhodamine WT dye was injected into the harbor near Ballybricken starting at 12:30 P.M. (BST) October 5, 1970 and terminating at 5:00 p.m. (BST) October 10, 1970. The injection rate was 0.44 gallons per hour and the concentration of the dye was 200,000 ppb. Figure 5.21 shows the location of the injection, which is the site where a diffuser for waste discharges was subsequently located. Dye concentrations were measured by a continuous reading fluorometer mounted on a boat

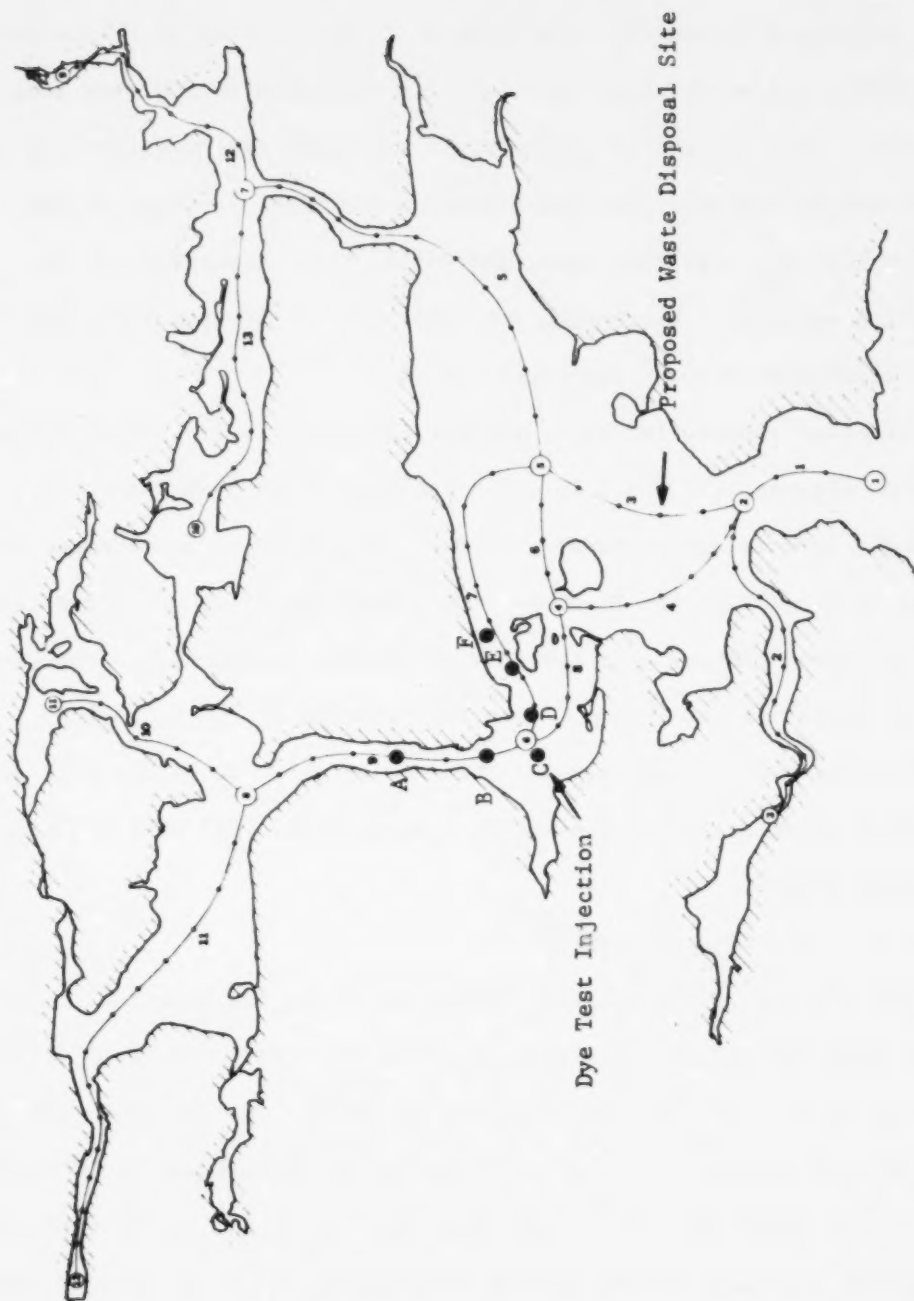


Figure 5.21 Vertical Profile Stations for Ballybricken Injection

which traversed the harbor at selected times during and after the time of injection. In addition to the traverses, vertical concentration profiles were taken at stations A,B,C,D,E, and F, which are shown in Figure 5.21.

No recordings of tidal stages were taken during the dye test; therefore, it is necessary to compute the tidal hydraulics using predicted heights from the Tide Tables. The predicted heights shown in Table 5.4 were used to generate a tide curve which was specified at node 1. Between the times of high water and low water, the tide curve was assumed to follow a cosine curve, as recommended by the Tide Tables. The computations were begun at early low tide on October 4, 1970 in order to provide a few tidal cycles for starting transients to die out before the beginning of the dye test.

The only information available on fresh water inflow was from a gaging station maintained by the Electric Supply Board in the River Lee at Leemount Bridge in Cork. Leemount Bridge is located downstream of Iniscarra Dam, and the gage data shows several sharp peaks in the river discharge which were apparently caused by releases for power generation. These peaks were ignored in the tidal hydraulics computations, and the base flows are summarized in Table 5.5.

Table 5.4 Predicted Tidal Stages for the Period of the Ballybricken Dye Test

Day	Hour	Feet Above MLW	Day	Hour	Feet Above MLW	Day	Hour	Feet Above MLW
10-4 SU	0219 0812 1435 2028	1.4 11.9 1.4 11.4	10-7 W	0408 1013 1640 2238	2.7 10.3 2.7 9.6	10-10 SA	0122 0805 1408 2047	9.0 3.0 9.7 2.5
10-5 M	0250 0847 1509 2103	1.7 11.5 1.8 10.9	10-8 TH	0508 1114 1751 2349	3.2 9.7 3.1 9.0	10-11 SU	0247 0922 1522 2153	9.7 2.1 10.6 1.5
10-6 TU	0325 0926 1549 2145	2.2 11.0 2.2 10.3	10-9 F	0632 1235 1922	3.4 9.3 3.1			

Table 5.5 Base Flows in the River Lee

Day	Flow (cfs)
10-4	353
10-5	371
10-6	388
10-7	417
10-8	395
10-9	388
10-10	392
10-11	385

As a simple estimate, a constant fresh water throughflow of 400 cfs was prescribed at Cork in the tidal hydraulics computations.

At the injection point, the tidal flow on ebb divides to flow around Haulbowline and Spike Islands. The dye was released on the water surface near the south side of the channel, and it was observed that the dye was swept into the narrow channel which passes between Haulbowline Island the the south shore. To reproduce this behavior in the mathematical model, the injection was placed 1400 feet below node 6 in reach 8. Parameters needed to set up the water quality computational mesh near the injection point were estimated from the hydraulic computations.

$$U \approx 1.0 \text{ ft/sec.} \quad (\text{maximum tidal velocity})$$

$$R_h \approx 15.0 \text{ ft.}$$

In the dye test simulation, the dispersion coefficient was taken as three

times the Taylor value, as in the James River Model study. Near the injection point,

$$E = 3 \cdot E_T \approx 54 \frac{\text{ft}^2}{\text{sec.}}$$

To enter the discretization criteria, a distance x is required for the parameter $\frac{Ux}{E}$. In network computations, a node often creates a sharp change in the concentration profiles as the discharge in one reach is diluted by flows in intersecting reaches. Therefore, the distance x is taken to be 1400 feet, and

$$\frac{Ux}{E} = 26$$

From Figure 3.6

$$(5\% \text{ cutoff}) = 1.0$$

The mesh spacing Δx is calculated as

$$\Delta x \leq \frac{4E}{U(5\% \text{ cutoff})} = 216 \text{ feet}$$

and the time step Δt is

$$\Delta t \leq \frac{\Delta x}{U} \leq 216 \text{ seconds.}$$

Near the injection point, the mesh spacing Δx was taken as 200 feet, and the time step was set at 294 seconds, which is the hydraulic time step. This corresponds to 150 time steps for the first tidal cycle beginning on October 4, 1970. Away from the injection point, the mesh spacing was gradually increased to as much as 2000 ft. in the upstream reaches.

A plot of computed and measured dye concentrations versus time at Stations D and B is shown in Figure 5.22. These two stations had the

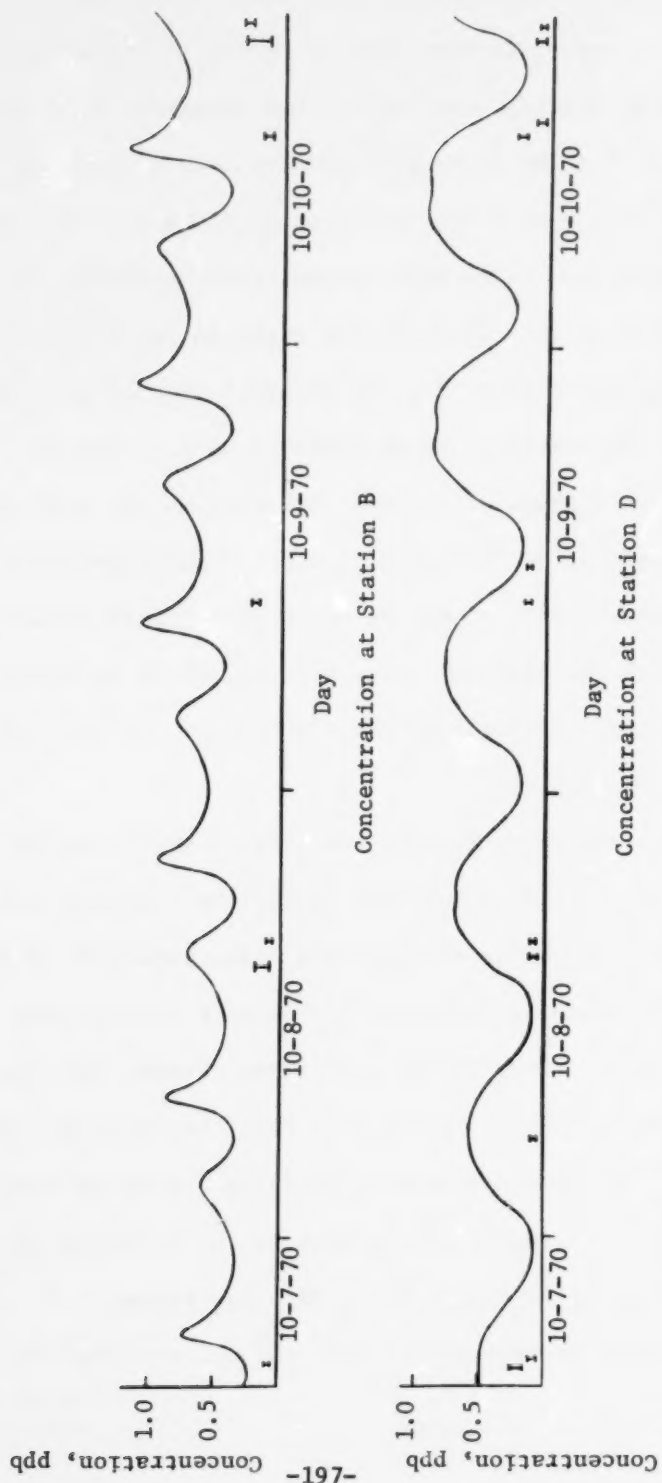


Figure 5.22 Dye Concentration versus Time at Stations B and D, Cork Harbour

most field measurements of dye concentration, which are quite sparsely distributed. Most of the measurements were taken within an hour or two of predicted low water, so they tend to define the troughs in the curves. Agreement at Station D is better than agreement at Station B, although it appears that the computed concentrations at both may be too high. A check of computed concentration profiles near the time of slack water showed that there were concentration gradients in the vicinity of Station B and D. Shifting the assigned locations of Station D and especially Station B a few thousand feet in the computations could change the resulting concentrations by a factor of 2. Schematization cannot reproduce the exact behavior of the prototype in the model; therefore, it is difficult to compare measurements at a point with computed results. Also, it may be noted that the field-measured concentrations are of the order of 0.1 - 0.2 ppb, which is rather close to the 0.03 ppb stated threshold of the fluorometer and the background concentration of 0.043 ppb.

No computations were made to test the effects of increasing dispersion, although it is likely that this would lower computed concentrations at Station B and D, which are within a tidal excursion of the injection. Holley, Harleman, and Fischer (1970) note that in some situations dispersion in estuary flow can be much larger than that predicted by the Taylor value. It was felt that the field data was too sparse to test the computations adequately, and computational effort was turned to the waste disposal simulations in the following section.

5.2.4 Simulation of Alternate Waste Disposal Schemes

Early work in Cork Harbour showed that the Ballybricken disposal

site would be inadequate for waste loads which were planned for the long term. To maintain water quality in the harbor within set standards, it was necessary to locate the disposal site closer to the harbor entrance. The increased tidal discharge provided greater dilution of the waste, and tidal flushing could be used to achieve removal from the harbor on ebb tide.

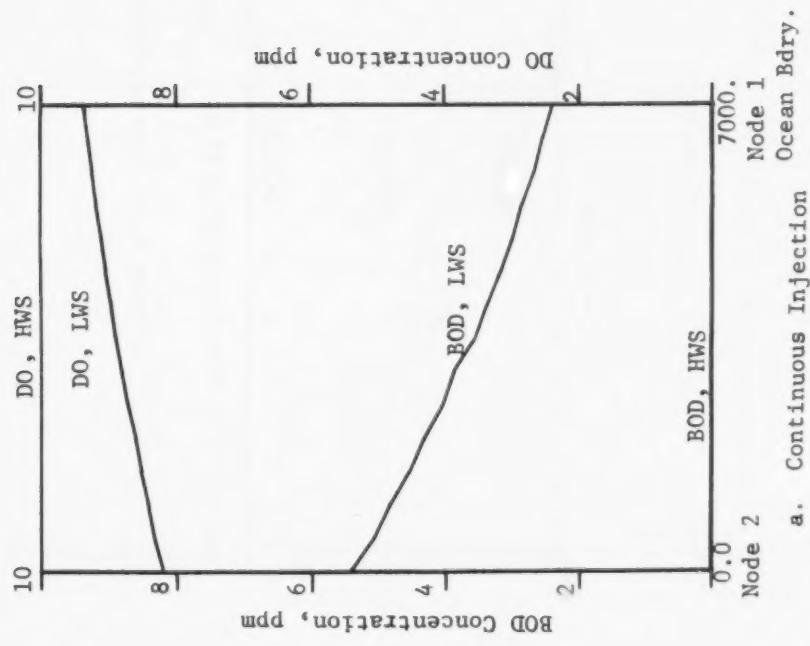
The purpose of this section is to demonstrate the ability of the mathematical model to handle waste disposal problems near the ocean boundary by simulating alternate injection schemes at a proposed site in reach 3 between nodes 5 and 2, as shown in Figure 5.21. The simulations were conducted using the 14-cycle transient tidal hydraulics which were computed for the Ballybricken dye study and stored on tape. During these 14 cycles, the tide range starts at about 10 feet, passes through a neap range of about 6 feet, and increases back to about 7 feet. Imposing transient hydraulics in this manner will result in more realistic concentration levels than if a single, steady-state, neap tidal cycle had been used. More waste will be lost to the ocean and dispersion will upread it further inside the harbor.

The level of waste load simulated was set at 470,000 lbs/day of BOD (ultimate), and its decay coefficient K_1 was taken to be 0.20 (base e). The reaeration coefficient K_2 was assigned a value of 0.23 (base e), and the saturation concentration of DO was assumed to be 10.0 ppm. At the ocean boundary, it was assumed that the transition of incoming water on flood tide to zero BOD and saturated DO was very fast. This results in negligible return of waste. Field studies are now underway in Cork

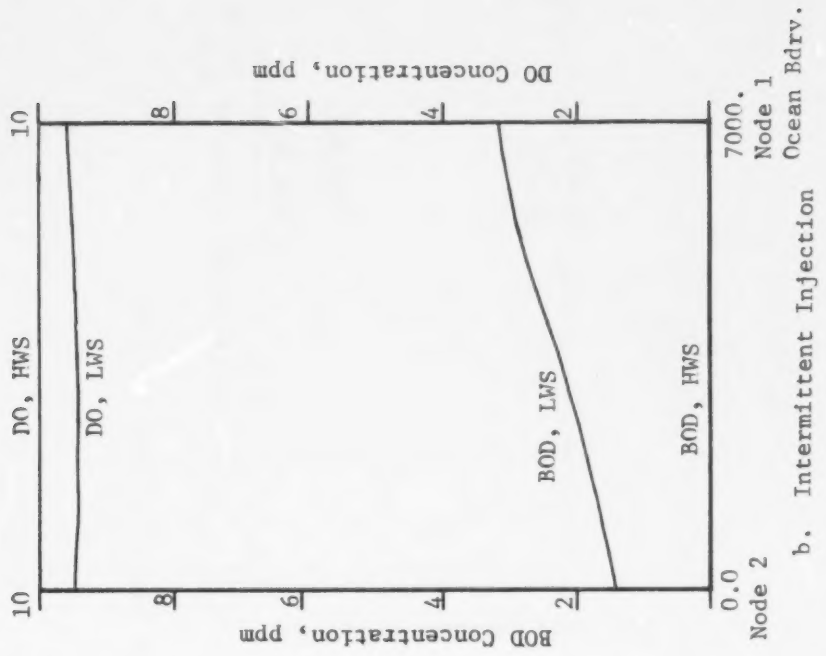
Harbour to estimate the per cent return, and the results can be used to refine the mathematical model when they are available. Selection of the water quality mesh was based on that used for the Ballybricken dye study where the mesh spacing started at 200 feet near the injection point and increased with distance away from it. To save computational time, the time step Δt was increased to 588 seconds or 75 steps per tidal cycle.

With injection continuous at the rate of 470,000 lbs/day of BOD, Figures 5.23a through 5.30a show the resulting BOD and DO profiles in reaches 1 through 8 at low water slack and high water slack of tidal cycle 14. The maximum BOD levels are approximately 6 ppm and the minimum DO concentrations are about 8 ppm, for a deficit of 2 ppm. It is interesting to note that there appears to be a "dead water" area in reach 6 between nodes 4 and 5 where BOD and DO concentrations appear to remain at maximum levels over the tidal cycle. This situation may exist physically, inasmuch as a "hot spot" of dye concentration was observed by field measurements in this area during the Ballybricken dye study.

The injection point is located within a tidal excursion of the ocean boundary, which may be observed in Figure 5.25a where clean water on flood tide has been marked by the injection. To place more of the waste in the water mass which leaves the estuary on ebb tide, it was decided to inject the waste intermittently during one quarter of the tidal period at a rate four times the continuous rate. The injection begins at the time of high water slack and proceeds for slightly more than three hours until the ebb velocity reaches its peak. This type of



a. Continuous Injection



b. Intermittent Injection

Figure 5.23 Concentration Profiles in Reach 1, Tidal Cycle 14

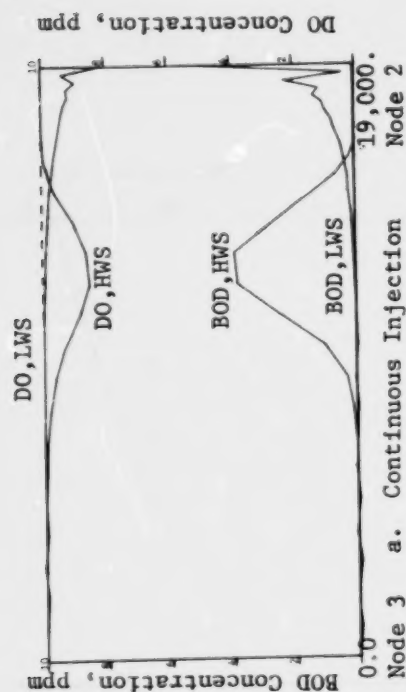
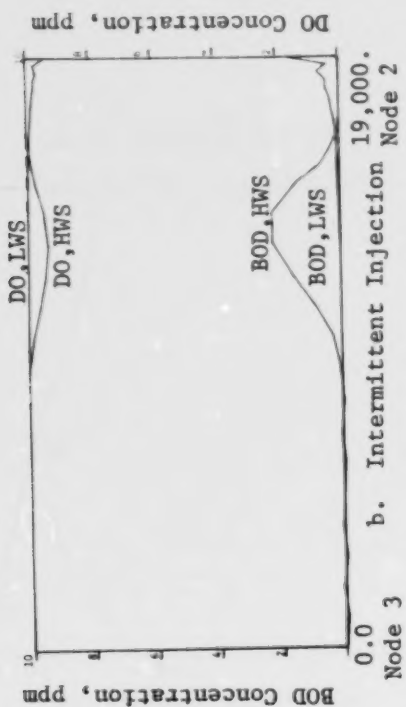


Figure 5.24 Concentration Profiles in Reach 2, Tidal Cycle 14

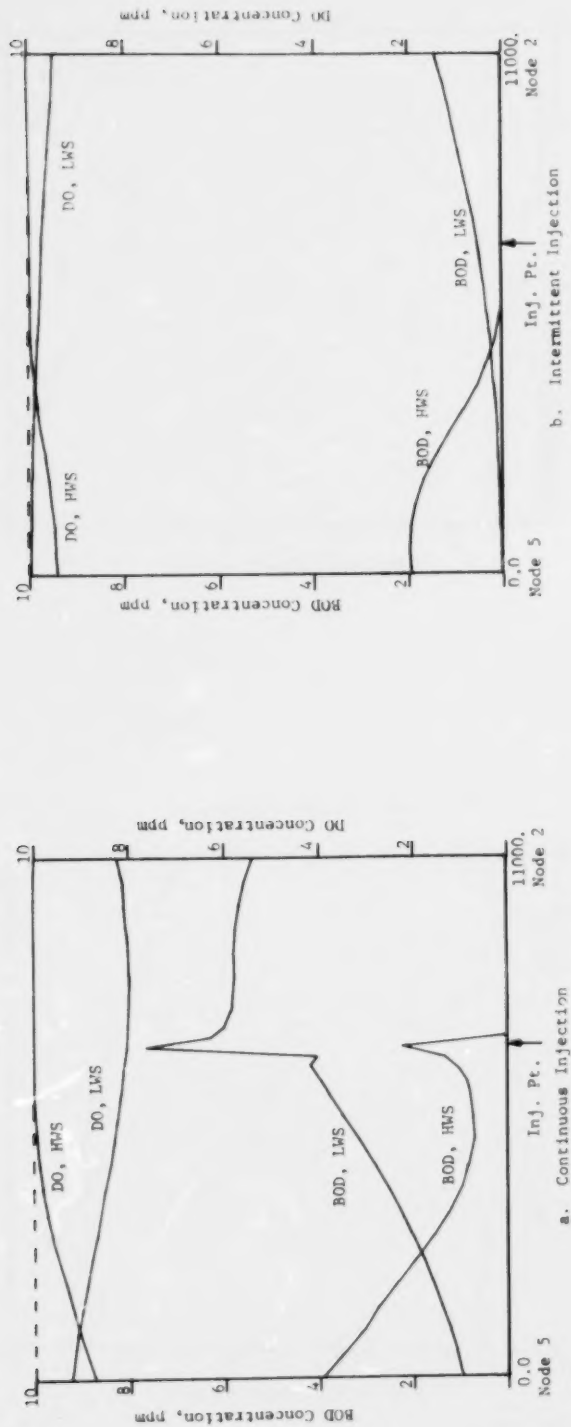


Figure 5.25 Concentration Profiles in Reach 3, Tidal Cycle 14

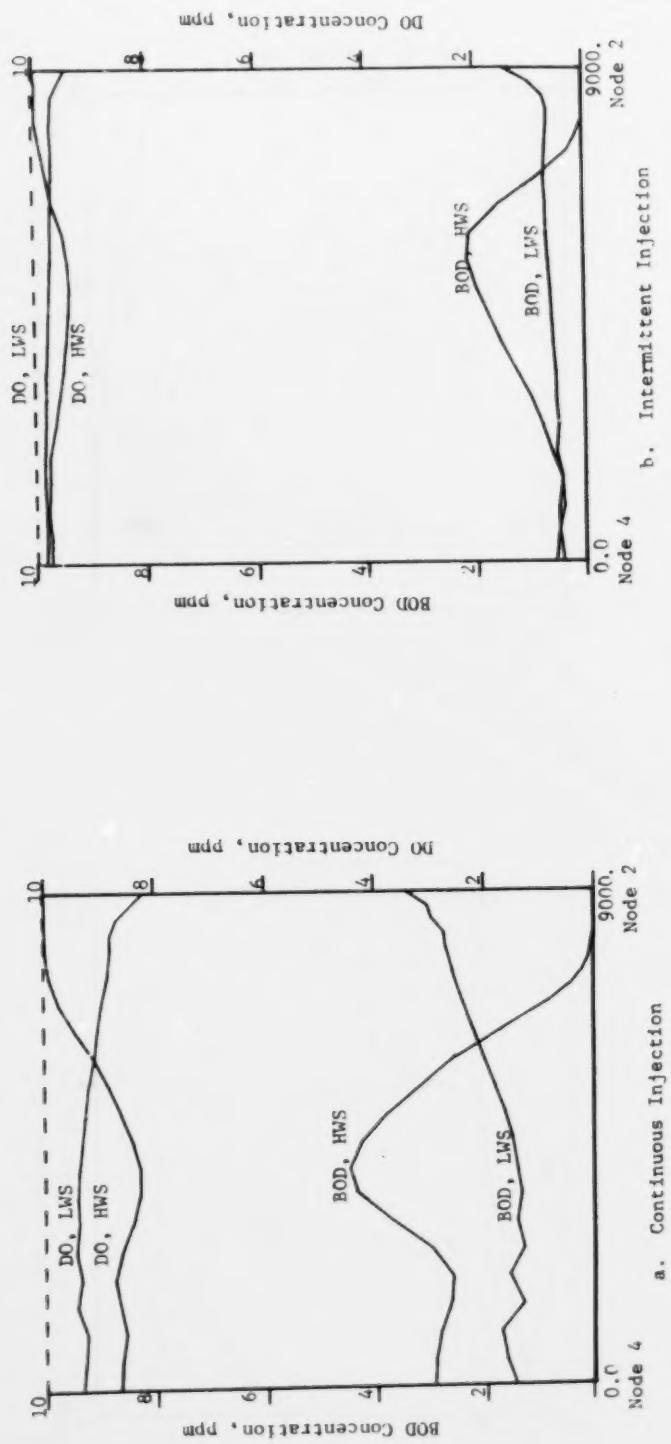


Figure 5.26 Concentration Profiles in Reach 4, Tidal Cycle 14

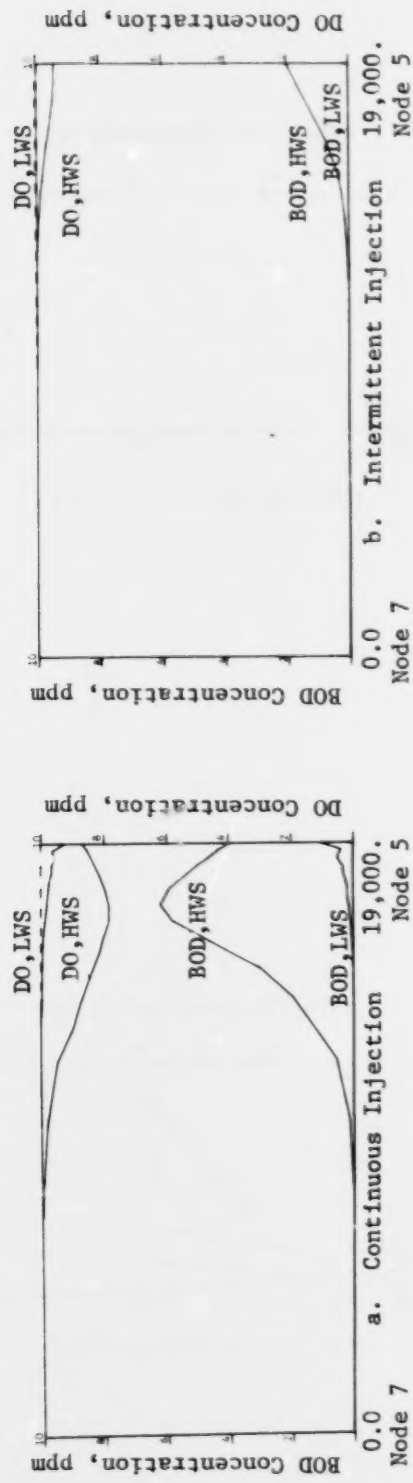
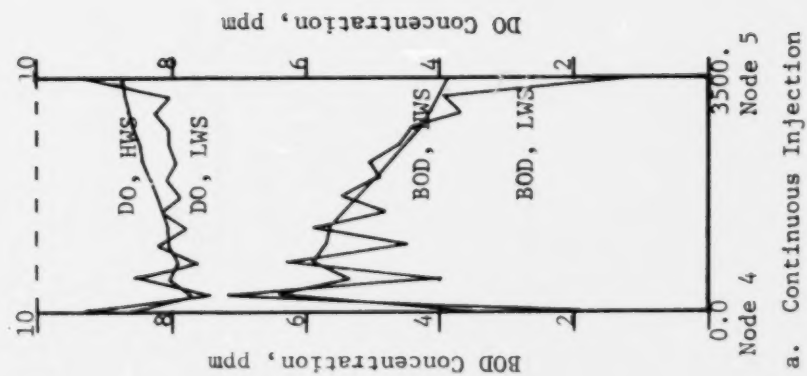
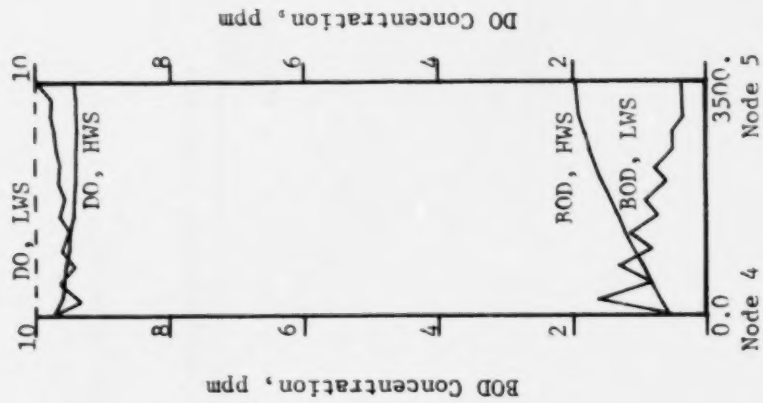


Figure 5.27 Concentration Profiles in Reach 5, Tidal Cycle 14



a. Continuous Injection



b. Intermittent Injection

Figure 5.28 Concentration Profiles in Reach 6, Tidal Cycle 14

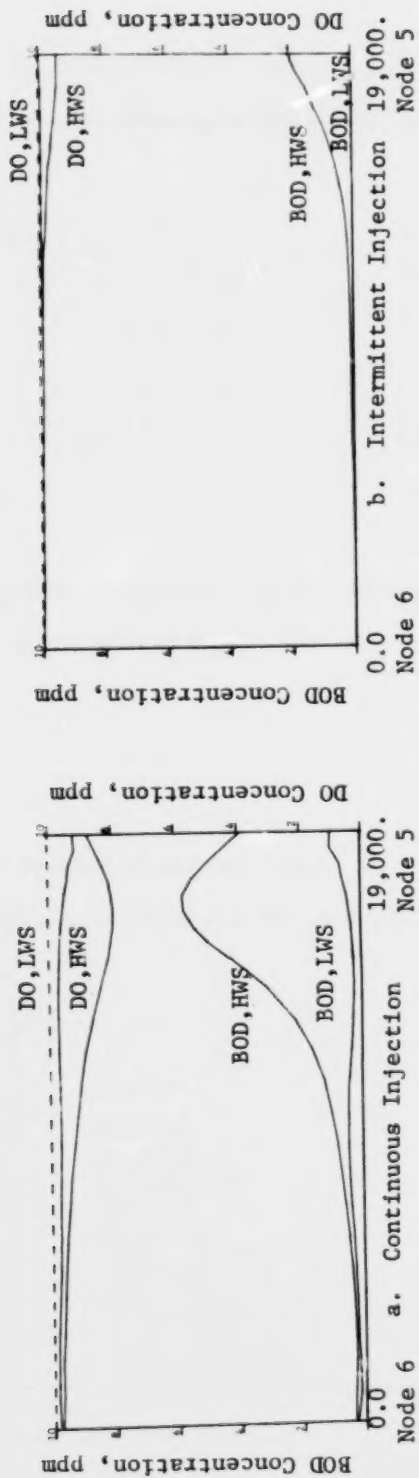
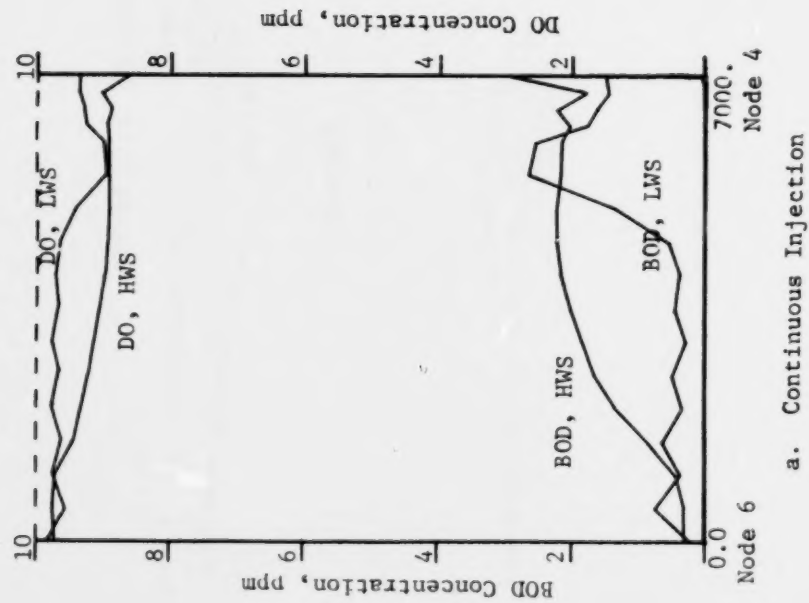
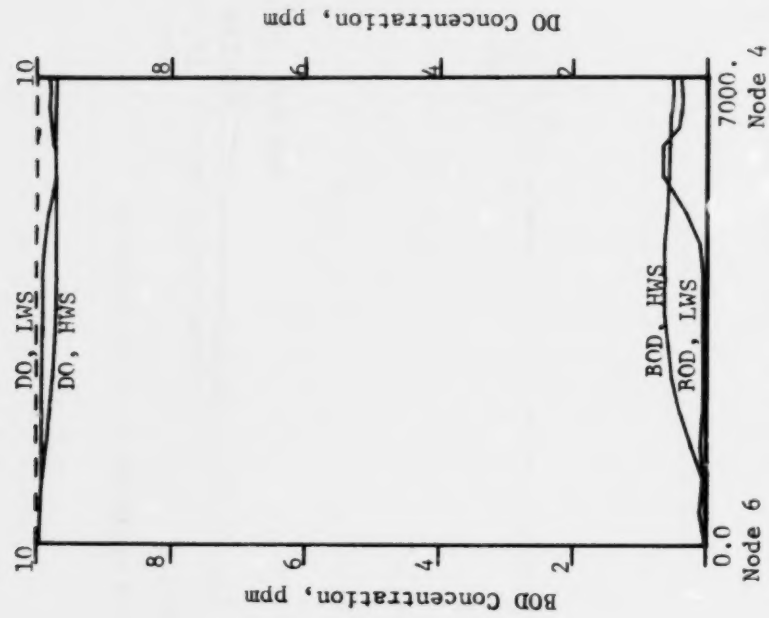


Figure 5.29 Concentration Profiles in Reach 7, Tidal Cycle 14



a. Continuous Injection



b. Intermittent Injection

Figure 5.30 Concentration Profiles in Reach 8, Tidal Cycle 14

schedule was feasible in this study because the wastes were generated in low volumes at high concentrations. Therefore, it is possible to detain the waste for three quarters of a tidal cycle.

The results of a simulation with waste injected during a quarter tidal cycle, intermittent schedule are shown in Figure 5.23b through 5.30b. Maximum BOD and DOD concentrations are approximately 2-3 ppm and 0.5 - 0.6 ppm, respectively. Therefore, the intermittent injection schedule has yielded a three-to four-fold improvement in the dissolved oxygen deficit in comparison with the continuous discharge. It is interesting to note in Figure 5.23b that the maximum BOD concentration occurs at the ocean boundary at low water slack. The concentration profile in reach 1 shows the trailing portion of a concentration peak which has passed through the ocean boundary. Moving the injection point closer to the ocean would displace this peak seaward and further reduce concentrations inside the estuary. This would also reduce the peak in reach 2 at high water slack which is swept in on the flood tide from reach 1.

CHAPTER VI

SUMMARY AND CONCLUSIONS

The objective of the study is the development of a predictive mathematical model for the transient distribution of water quality constituents in an estuary which can be described as a network of branched and looped, one-dimensional channels. The time scale used in the mathematical model is on the order of minutes, which is much smaller than a tidal period, but greater than that of turbulent fluctuations. It is important to use "tidal time" when simulating the longitudinal dispersion and tidal flushing near the ocean boundary. Four constituents are included in the mathematical model; salinity, temperature, BOD, and DO.

To be predictive, a mathematical water quality model must correctly reproduce both the transport processes by which a constituent is advected and dispersed, and the reaction processes by which mass of constituent is added to, or removed from the system. In this study, the reaction processes are considered to be characterized by first-order reaction kinetics. Complex, non-linear reactions could be handled by varying the reaction coefficient at each time step in the computations to reflect a functional dependence on other water quality constituents and external conditions.

The transport processes are based on a combined solution of the continuity and momentum equations. This solution is subject to the boundary conditions that a known tide curve is prescribed at the ocean boundary and that the discharge (hence, the momentum flux) at a head of

tide is zero. Fresh water inflow at a head of tide is included as a tributary inflow. The continuity and momentum equations provide discharges and water surface elevations which define the storage and advective terms in a conservation of mass equation for each constituent. The longitudinal dispersion term is based on the studies of Thatcher and Harleman who combined the dispersion induced by the salinity intrusion with the dispersion resulting from the shear induced cross-sectional velocity distribution.

To solve the conservation of mass equation for the various constituents, it is necessary to prescribe boundary conditions. At an upstream boundary, mass flux into the system is specified. At the ocean entrance, the boundary condition is divided into two parts, depending on the direction of the tidal flow. On ebb tide, the transport of mass across the ocean boundary is determined by seaward advective flow and the concentration distribution within the estuary. On flood tide, the concentration of inflowing water at the ocean boundary is prescribed.

The numerical solution of the continuity, momentum, and conservation of mass equations is based on the method of weighted residuals, which is an application technique of the finite element method. For a branched and looped network, the method of weighted residuals has several advantages over other numerical solution techniques such as finite difference methods. Solutions for the individual channels in a network can be matched conveniently at the intersections, or nodes. Also, the mesh spacing between grid points along the axis of a channel can be

variable rather than fixed, as in finite difference methods. This feature is useful in the vicinity of steep concentration gradients where the mesh can be refined to resolve the concentration profile.

Discretization criteria have been developed to choose the mesh spacing Δx and the time step Δt , based on values of the advective velocity U , the longitudinal dispersion coefficient E , and the decay coefficient K . The discretization criteria were tested by computing numerical solutions of simplified problems for which analytical solutions were available. Agreement of the numerical and analytical solutions was excellent.

The predictive capability of the network water quality model was demonstrated by simulating dye studies conducted in the James River Model at the U.S. Army Corps of Engineers Waterways Experiment Station. Dye (if conservative) is a useful substance to test the capability of a mathematical model to predict the advective and dispersive processes since it eliminates concern with estimating decay coefficients. The hydraulic model tests were simulated because they were conducted under conditions which could be reproduced easily in the mathematical model and because the data was extensive and reliable. Computed results agreed well with measured concentrations. The model dye test results showed that transient water quality phenomena such as the movement of dye fronts are very sensitive to dispersion. The agreement with measured concentrations was achieved with a Taylor dispersion coefficient which was increased slightly to account for natural irregularities in the channels. An additional test which simulated a large increase in

the dispersion coefficient resulted in a marked distortion of the concentration profiles.

The mathematical model was also used to study water quality in Cork Harbour, Ireland. Initially, the model was used to simulate a dye test conducted by Metcalf and Eddy, Inc. within the harbor. Although computed results and measured concentrations were in qualitative agreement, sparse field data made it difficult to draw quantitative conclusions.

An earlier study of Cork Harbour showed that water quality standards under planned, long-term waste loadings could be maintained by taking advantage of the natural tidal flushing. The network mathematical model developed in this study was used to investigate alternate waste discharge schemes at a proposed injection site approximately two miles from the ocean entrance. A comparison was made of the distribution of BOD and DO for a continuous injection and for an intermittent injection. In the intermittent injection scheme wastes were discharged during one quarter of the tidal period, on the ebb tide following high water slack, at four times the continuous rate. The intermittent injection yielded significant reductions in BOD and DOD levels within the harbor.

REFERENCES

- Arons, A.B. and Stommel, H. (1951), "A Mixing Length Theory of Tidal Flushing", Transactions, American Geophysical Union, Vol. 32, No. 3, June, 1951, pp. 419-421.
- Boland, R.A. (1972), "Private Communications", U. S. Army Corps of Engineers Waterways Experiment Station, Vicksburg, Mississippi.
- Clark, L.J. and Feigner, K.D. (1972), "Mathematical Model Studies of Water Quality in the Potomac Estuary", Tech. Rep. 33, Annapolis Field Office, Region III, Environmental Protection Agency, March, 1972.
- Cook, D.O. (1972), "Private Communications", Submarine Signal Division, Raytheon Co., Portsmouth, Rhode Island.
- Crandall, S.H. (1956), Engineering Analysis, McGraw-Hill, New York, New York, 1956.
- Di Toro, D.M. (1972), "Recurrence Relations for First Order Sequential Reactions in Natural Waters", Water Resources Research, Vol. 8, No. 1, February, 1972, pp. 50-57.
- Feigner, K.D. and Harris, H.S. (1970), "Documentation Report, FWQA Dynamic Estuary Model", U. S. Department of the Interior, Federal Water Quality Administration, July, 1970.
- Fischer, H.B. (1969), "A Lagrangian Method for Predicting Pollutant Transport in Bolinas Lagoon, California", U. S. Geological Survey Open File Report, Menlo Park, California, December, 1969.
- Fischer, H.B. (1970), "A Method for Predicting Pollutant Transport in Tidal Waters", Water Resources Center Contribution No. 132, Hydr. Engrg. Lab., University of California, Berkeley, March, 1970.
- Fisher, J.S., Nava, R.E. and Cross, R.H. (1971), "Mathematical Model of the Maracaibo Estuary", Tech. Rep. No. 136, Ralph M. Parsons Laboratory, Massachusetts Institute of Technology, February, 1971.
- FWQA (1968), "Prototype and Hydraulic Dye Test Data for James River", James River Study Project, FWQA Charlottesville Regional Office, Charlottesville, Virginia (unpublished).
- Gilcrest, B.R. (1958), Chapter X, Engineering Hydraulics, Edited by H. Rouse, John Wiley & Sons, New York, New York, 1958.
- Gunaratnum, D.J. and Perkins, F.E., "Numerical Solution of Unsteady Flows in Ocean Channels", Tech. Rep. No. 127, Hydrodynamics Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, July, 1970.

- Guymon, G.L. (1970), "A Finite Element Solution of the One-Dimensional Diffusion-Convection Equation", Water Resources Research, Vol. 6, No. 1, February, 1970, pp. 204-210.
- Harleman, D.R.F., Holley, Jr., E.R. and Huber, W.C. (1966), "Interpretation of Water Pollution Data from Tidal Estuary Models", Third International Conference on Water Pollution Research, Munich, Germany, 1966.
- Harleman, D.R.F. and Lee, C.H. (1969), "The Computation of Tides and Currents in Estuaries and Canals", Technical Bulletin No. 16, Committee on Tidal Hydraulics, U.S. Army Corps of Engineers, September, 1969.
- Holley, Jr., E.R. and Harleman, D.R.F. (1965), "Dispersion of Pollutants in Estuary Type Flows", Tech. Rep. No. 74, Hydrodynamics Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, January, 1965.
- Holley, Jr., E.R., Harleman, D.R.F. and Fischer, H.B. (1970), "Dispersion in Homogeneous Estuary Flow", Journal of the Hydraulics Division, ASCE, Vol. 96, No. HY8, August, 1970, pp. 1691-1709.
- Lai, Chintu (1965), "Flows of Homogeneous Density in Tidal Reaches, Solution by Implicit Method", U.S. Geological Survey Open File Report, Washington, D.C., 1965.
- Lai, Chintu (1967), "Computation of Transient Flows in Rivers and Estuaries by the Multiple-Reach Method of Characteristics", U.S. Geological Survey Professional Paper 575D, 1967, pp. D273-D280.
- Lee, C.H. and Harleman, D.R.F. (1971), "One-Dimensional, Real-Time Model for Estuarine Water Quality Prediction", Report 16070 DGW, Water Quality Office, Environmental Protection Agency, Washington, D.C., (in press).
- Leendertse, J.J. and Gritton, E.C. (1971), "A Water Quality Simulation Model for Well Mixed Estuaries and Coastal Seas: Vol. II, Computation Procedures", Tech. Rep. R-708-NYC, The New York City-Rand Institute, New York, New York, July, 1971.
- Leendertse, J.J. and Gritton, E.C. (1971), "A Water Quality Simulation Model for Well-Mixed Estuaries and Coastal Seas: Vol. III, Jamaica Bay Simulation", Tech. Rep. R-709-NYC, The New York City-Rand Institute, New York, New York, July, 1971.
- Metcalf and Eddy, Inc. (1971), "Report to Pfizer International Inc. on Disposal of Liquid Wastes in Cork Harbour, Ireland", Boston Massachusetts, April, 1970.

- O'Connor, D.J. (1965), "Estuarine Distribution of Non-Conservative Substances", Journal of the Sanitary Division, ASCE, Vol. 91, No. SA1, February, 1965, pp. 23-42.
- O'Kane, J.P.J. (1968), "A Prediction Model for the Pollution of the Lee Estuary", M. Eng. Sc. Thesis, National University of Ireland, Cork, 1968.
- Okubo, A. (1964), "Equations Describing the Diffusion of an Introduced Pollutant in a One-Dimensional Estuary", Studies in Oceanography, University of Tokyo Press, pp. 216-226.
- Parker, D.S., Norris, D.P. and Nelson, A.W. (1972), "Tidal Exchange at Golden Gate", Journal of the Sanitary Division, ASCE, Vol. 98, No. 2, April, 1972, pp. 305-323.
- Price, H.S., Cavendish, J.C. and Varga, P.S. (1968), "Numerical Methods of Higher Order Accuracy for Diffusion Convection Equations", Journal of the Society of Petroleum Engineers, September, 1968, pp. 293-303.
- Ryther, J.H. (1971), "Recycling Human Wastes to Enhance Food Production from the Sea", Environmental Letters, Vol. 1, No. 2, 1971, pp. 79-87.
- Shankar, N.J. and Masch, F.D. (1970), "Influence of Tidal Inlets on Salinity and Related Phenomena in Estuaries", Tech. Rep. HYD-16-7001, Hydr. Engrg. Lab., Department of Civil Engineering, University of Texas, Austin, March, 1970.
- Sherman, R.G. (1972), "Private Communications", Metcalf and Eddy, Inc., Boston, Massachusetts.
- Stommel, H. (1953), "Computation of Pollution in a Vertically Mixed Estuary", Sewage and Industrial Wastes, Vol. 25, No. 9, September, 1953, pp. 1065-1071.
- Stone, H.L. and Brian, P.L.T. (1963), "Numerical Solution of Convective Transport Problems", Journal of the American Institute of Chemical Engineers, Vol. 9, No. 5, September, 1963, pp. 681-688.
- Thatcher, M.L. and Harleman, D.R.F. (1972), "A Mathematical Model for the Prediction of Unsteady Salinity Intrusion in Estuaries", Tech. Rep. No. 144, Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, February, 1972.
- Thomann, R.V. (1963), "Mathematical Model for Dissolved Oxygen", Journal of the Sanitary Division, ASCE, Vol. 89, No. SA5, October, 1963, pp. 1-30.

Tide Tables, Revised Annually, National Ocean Survey (formerly U.S. Coast and Geodetic Survey), Department of Commerce, Washington, D.C.

TRACOR (1971), Estuarine Modeling: An Assessment, Water Quality Office, Environmental Protection Agency, February, 1971.

Wicker, C.F. (1955), "The Prototype and Model Delaware Estuary", Proceedings of the Sixth Congress of the I.A.H.R., Vol. 1, The Hague, pp. A12-1 - A12-18, 1955.

Wood, E.F., Harley, B.M. and Perkins, F.E. (1972), "Operational Characteristics of a Numerical Solution for the Simulation of Open Channel Flow", Tech. Rep. No. 150, Ralph M. Parsons Laboratory, Department of Civil Engineering, Massachusetts Institute of Technology, June, 1972.

Zienkiewicz, O.C. and Cheung, Y.K. (1967), The Finite Element Method in Structural and Continuum Mechanics, McGraw-Hill, New York, New York, 1967.

Zienkiewicz, O.C. and Parekh, C.J. (1970), "Transient Field Problems: Two-Dimensional and Three-Dimensional Analysis by Isoparametric Finite Elements", International Journal for Numerical Methods in Engineering, Vol. 2, No. 1, March, 1970, pp. 61-71.

APPENDIX A

SUMMARY OF INTEGRAL VALUES IN THE WEIGHTED RESIDUAL EQUATIONS

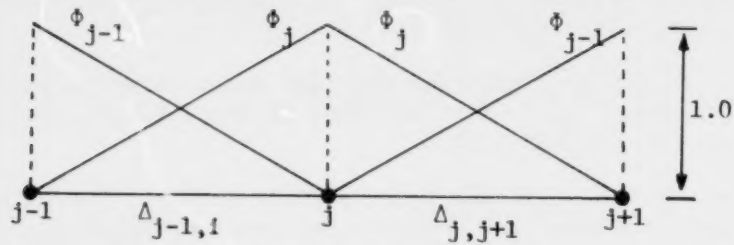


Figure A.1 Interpolating Functions in Adjacent Elements

In Element $j-1,j$:

$$\phi_{j-1} = \frac{x_j - x}{\Delta_{j-1,j}}$$

$$\phi_j = \frac{-x_{j-1} + x}{\Delta_{j-1,j}}$$

$$\phi_{j+1} = 0$$

In Element $j,j+1$:

$$\phi_{j-1} = 0$$

$$\phi_j = \frac{x_{j+1} - x}{\Delta_{j,j+1}}$$

$$\phi_{j+1} = \frac{-x_j + x}{\Delta_{j,j+1}}$$

Only in elements $j-1, j$ and $j, j+1$ will integrals containing ϕ_j provide a non-zero contribution. Their values are as follows:

$$\sum_E \int \frac{d\phi_j}{dx} \frac{d\phi_{j-1}}{dx} dx = -\frac{1}{\Delta_{j-1,j}}$$

$$\sum_E \int \frac{d\phi_j}{dx} \frac{d\phi_j}{dx} dx = \frac{1}{\Delta_{j-1,j}} + \frac{1}{\Delta_{j,j+1}}$$

$$\sum_E \int \frac{d\phi_j}{dx} \frac{d\phi_{j+1}}{dx} dx = -\frac{1}{\Delta_{j,j+1}}$$

$$\sum_E \int \phi_j \frac{d\phi_{j-1}}{dx} dx = -\frac{1}{2}$$

$$\sum_E \int \phi_j \frac{d\phi_j}{dx} dx = 0$$

$$\sum_E \int \phi_j \frac{d\phi_{j+1}}{dx} dx = \frac{1}{2}$$

$$\sum_E \int \frac{d\phi_j}{dx} \phi_{j-1} dx = \frac{1}{2}$$

$$\sum_E \int \frac{d\phi_j}{dx} \phi_{j+1} dx = -\frac{1}{2}$$

$$\sum_E \int \phi_j \phi_{j-1} dx = \frac{\Delta_{j-1,j}}{6}$$

$$\sum_E \int \phi_j \phi_j dx = \frac{\Delta_{j-1,j}}{3} + \frac{\Delta_{j,j+1}}{3}$$

$$\sum_E \int \phi_j \phi_{j+1} dx = \frac{\Delta_{j,j+1}}{6}$$

APPENDIX B

SPECTRAL DENSITY OF THE CONCENTRATION RESPONSE TO AN INSTANTANEOUS INJECTION OF MASS

The linear system is defined by the convective diffusion equation including decay and source terms.

$$\frac{\partial c}{\partial t} + U \frac{\partial c}{\partial x} = E \frac{\partial^2 c}{\partial x^2} - Kc + (\text{source term}) \quad (1)$$

The spectral density of the impulse response for an instantaneous injection of unit mass is

$$S(\sigma, x) = |H(\sigma, x)|^2 \quad (2)$$

where

$S(\sigma, x)$ = spectral density as a function of angular frequency $\sigma = \frac{2\pi}{T}$
and distance x

$H(\sigma, x)$ = complex frequency response

To evaluate the complex frequency response, consider an excitation in Equation (1) which is due to a point source oscillating in time at the origin $x = 0$.

$$(\text{source term}) = \delta(x)e^{i\sigma t} \quad (3)$$

The concentration response will be

$$c = H(\sigma, x)e^{i\sigma t} \quad (4)$$

It may be recalled from the Fourier series solution of the convective diffusion equation that all harmonics propagate through the system at velocity U . Therefore,

$$\sigma = \omega U \quad (5)$$

Continuing to work in terms of σ , Equations (3) and (4) are substituted into Equation (1). After cancelling the exponential terms,

$$i\sigma H + U \frac{dH}{dx} = E \frac{d^2 H}{dx^2} - KH + \delta(x) \quad (6)$$

The homogeneous form of Equation (6) can be satisfied by the exponential substitution

$$H = Ae^{\lambda x} \quad (7)$$

The characteristic equation is

$$(i\sigma + K) + \lambda U - \lambda^2 E = 0 \quad (8)$$

Solving for the exponent λ ,

$$\lambda = \frac{U}{2E} \left\{ 1 \pm \sqrt{\left(1 + \frac{4KE}{U^2}\right) + i \frac{4\sigma E}{U^2}} \right\} \quad (9)$$

The complex number under the radical can be expressed as

$$\sqrt{\left(1 + \frac{4KE}{U^2}\right) + i \frac{4\sigma E}{U^2}} = re^{i\theta} \quad (10)$$

where

$$r = \left[\left(1 + \frac{4KE}{U^2}\right)^2 + \left(\frac{4\sigma E}{U^2}\right)^2 \right]^{1/4}$$

$$\theta = \frac{1}{2} \tan^{-1} \left(\frac{\frac{4\sigma E}{U^2}}{1 + \frac{4KE}{U^2}} \right)$$

With these definitions, the homogeneous solution for $H(\sigma, x)$ can be written:

$$H(\sigma, x) = A_1 e^{\lambda_1 x} + A_2 e^{\lambda_2 x} \quad (11)$$

where

$$\lambda_1 = \frac{U}{2E} \{1 + re^{i\theta}\} = \frac{U}{2E} \{1 + r \cos\theta\} + i \frac{U}{2E} \{r \sin\theta\}$$

$$\lambda_2 = \frac{U}{2E} \{1 - re^{i\theta}\} = \frac{U}{2E} \{1 + r \cos\theta\} - i \frac{U}{2E} \{r \sin\theta\}$$

The real parts of λ_1 and λ_2 must be investigated to insure that $H(\sigma, x)$ remains finite as $x \rightarrow \pm \infty$. Figure B.1 shows that $r \cos\theta \geq 1$ for all values of $\frac{4\sigma E}{U^2}$ and $\frac{4KE}{U^2}$. Therefore, it is necessary to take $A_1 = 0$ for $x > 0$ and $A_2 = 0$ for $x < 0$. The homogeneous solution is written for two solution domains:

$$H(\sigma, x) = A_2 e^{\frac{Ux}{2E} \{1 - re^{i\theta}\}}, \quad x > 0 \quad (12a)$$

$$H(\sigma, x) = A_1 e^{\frac{Ux}{2E} \{1 + re^{i\theta}\}}, \quad x < 0 \quad (12b)$$

A complete solution for $H(\sigma, x)$ can be obtained by imposing the two conditions that (i) $H(\sigma, x)$ is continuous across the source at $x = 0$, and (ii) mass flux is conserved across the source. Applying the first condition near the origin:

$$H(\sigma, 0+) = A_2 \quad (13a)$$

and

$$H(\sigma, 0-) = A_1 \quad (13b)$$



Figure B.1 Evaluation of $r \cos \theta$ as a Function of $\frac{4cE}{U^2}$ and $\frac{4KE}{U^2}$

Therefore,

$$A_1 = A_2 \quad (14)$$

An expression for conservation of mass across the source may be obtained by integrating Equation (6) from $-\epsilon$ to $+\epsilon$:

$$(i\sigma + K) \int_{-\epsilon}^{+\epsilon} H dx + U \int_{-\epsilon}^{+\epsilon} \frac{dH}{dx} dx - E \int_{-\epsilon}^{+\epsilon} \frac{d^2 H}{dx^2} dx = \int_{-\epsilon}^{+\epsilon} \delta(x) dx \quad (15a)$$

or

$$(i\sigma + K) \left[H dx + UH \right]_{-\epsilon}^{+\epsilon} - E \left[\frac{dH}{dx} \right]_{-\epsilon}^{+\epsilon} = 1 \quad (15b)$$

As $\epsilon \rightarrow 0$, Equation (15) reduces to

$$\left. \frac{dH}{dx} \right|_{0+} - \left. \frac{dH}{dx} \right|_{0-} = -\frac{1}{E} \quad (16)$$

From Equation (12),

$$\left. \frac{dH}{dx} \right|_{0+} = A_2 \frac{U}{2E} [1 - re^{i\theta}] \quad (17a)$$

$$\left. \frac{dH}{dx} \right|_{0-} = A_1 \frac{U}{2E} [1 + re^{i\theta}] \quad (17b)$$

Recalling that $A_1 = A_2$ and substituting Equations (17) into Equation (16) yields the result

$$A_1 = A_2 = \frac{1}{Ure^{i\theta}} \quad (18)$$

Therefore, the complete solution for the complex frequency response is:

$$H(\sigma, x) = \frac{1}{U r e^{i\theta}} e^{\frac{Ux}{2E} [1 - r e^{i\theta}]}, \quad x > 0 \quad (19a)$$

$$H(\sigma, x) = \frac{1}{U r e^{i\theta}} e^{\frac{Ux}{2E} [1 + r e^{i\theta}]}, \quad x < 0 \quad (19b)$$

The spectral density $S(\sigma, x)$ is determined by substituting Equations (19) into Equation (2). For practical application, only the region downstream of the injection point will be considered. The result is:

$$S(\sigma, x) = \frac{1}{U^2 r^2} e^{\frac{Ux}{E} [1 - r \cos \theta]}, \quad x > 0 \quad (20)$$

It is often useful to have the normalized spectral density which is defined as

$${}^0S(\sigma, x) = \frac{S(\sigma, x)}{S(0, x)} \quad (21)$$

For $\sigma = 0$, the following results hold:

$$\theta = 0 \quad (22a)$$

$$\cos \theta = 1 \quad (22b)$$

and

$$r = r_o = \sqrt{\frac{4KE}{1 + U^2}} \quad (22c)$$

Therefore,

$$S(0, x) = \frac{1}{U^2 r_o^2} e^{\frac{Ux}{E} [1 - r_o]} \quad (23)$$

Substituting Equations (5), (20) and (23) into Equation (21), the normalized spectral density becomes

$$\phi_S(\omega, x) = \left(\frac{r_0}{r}\right)^2 e^{[r_0 - r \cos \theta] \frac{Ux}{E}}, \quad x > 0 \quad (24)$$

where

$$r = \left[\left(1 + \frac{4KE}{U^2}\right)^2 + \left(\frac{4\omega E}{U}\right)^2 \right]^{1/4}$$

and

$$\theta = \frac{1}{2} \tan^{-1} \left(\frac{\frac{4\omega E}{U}}{1 + \frac{4KE}{U^2}} \right)$$